Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (XH +) 0.44 ±0.03 (n=50)
logP (neutral X) 3.29 ±0.01 (n=50)

18B-28011 Points 1 to 22

M07_octanol concentration factor 1.039
Carbonate 0.1202 mM
Acidity error 0.21327 mM

18B-28011 Points 23 to 45

M07_octanol concentration factor 1.041
Carbonate 0.1876 mM
Acidity error 0.19535 mM

18B-28011 Points 46 to 79

M07_octanol concentration factor 0.988
Carbonate 0.1406 mM
Acidity error 2.18588 mM

Warnings and errors

Errors None
Warnings None

Sample logD and percent species

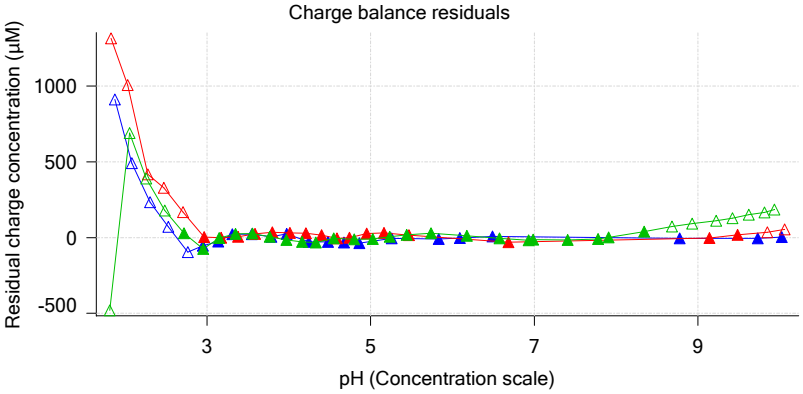
pH	M07_octanol logD	M07_octanol M07_octanolH	M07_octanol M07_octanol	M07_octanol M07_octanolH*	M07_octanol M07_octanol*	Comment
1.000	0.45	26.38 %	0.00 %	73.19 %	0.43 %	
1.200	0.45	26.31 %	0.00 %	73.00 %	0.69 %	Stomach pH
2.000	0.47	25.38 %	0.00 %	70.44 %	4.18 %	
3.000	0.65	18.44 %	0.02 %	51.18 %	30.36 %	
4.000	1.28	4.94 %	0.04 %	13.70 %	81.31 %	
5.000	2.19	0.59 %	0.05 %	1.65 %	97.71 %	
6.000	2.95	0.06 %	0.05 %	0.17 %	99.72 %	
6.500	3.15	0.02 %	0.05 %	0.05 %	99.88 %	
7.000	3.24	0.01 %	0.05 %	0.02 %	99.93 %	
7.400	3.27	0.00 %	0.05 %	0.01 %	99.94 %	Blood pH
8.000	3.28	0.00 %	0.05 %	0.00 %	99.95 %	
9.000	3.29	0.00 %	0.05 %	0.00 %	99.95 %	
10.000	3.29	0.00 %	0.05 %	0.00 %	99.95 %	
11.000	3.29	0.00 %	0.05 %	0.00 %	99.95 %	
12.000	3.29	0.00 %	0.05 %	0.00 %	99.95 %	

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

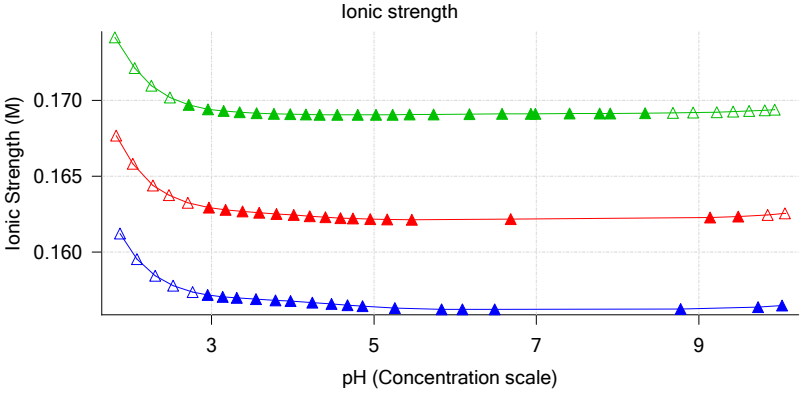
Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs

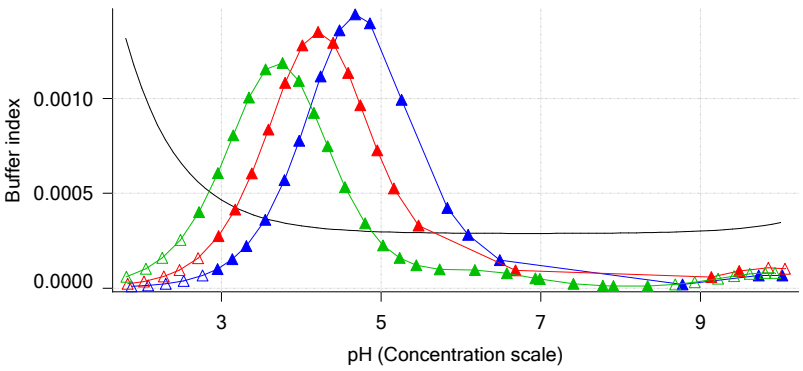
Charge balance residuals



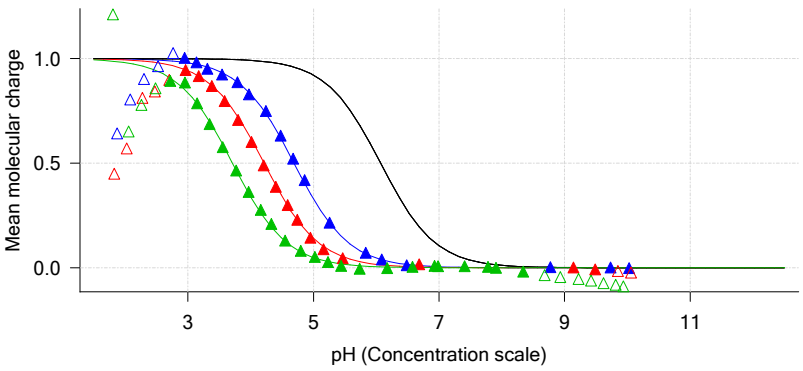
Ionic strength



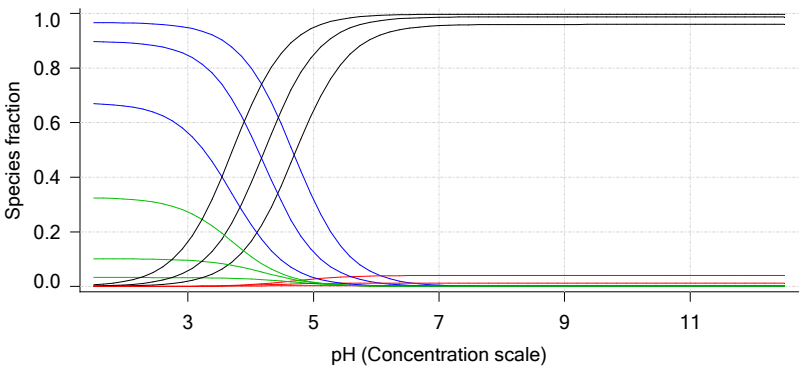
Buffer index profile



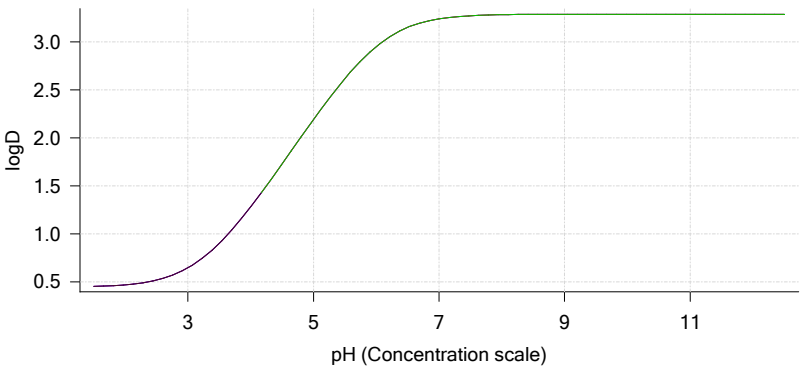
Sample M07_octanol Ionisation Graph



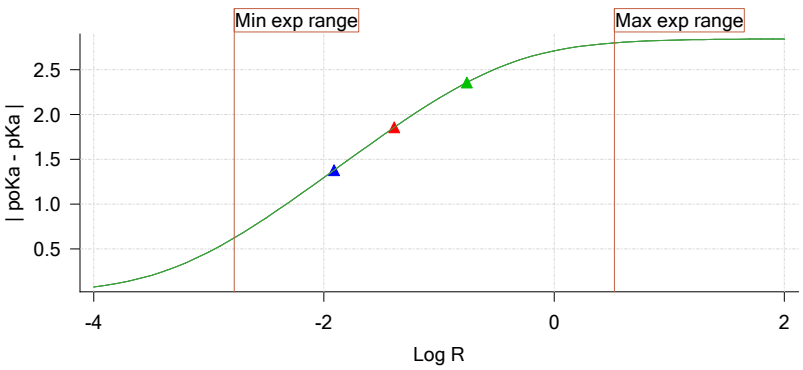
Distribution of species for sample M07_octanol



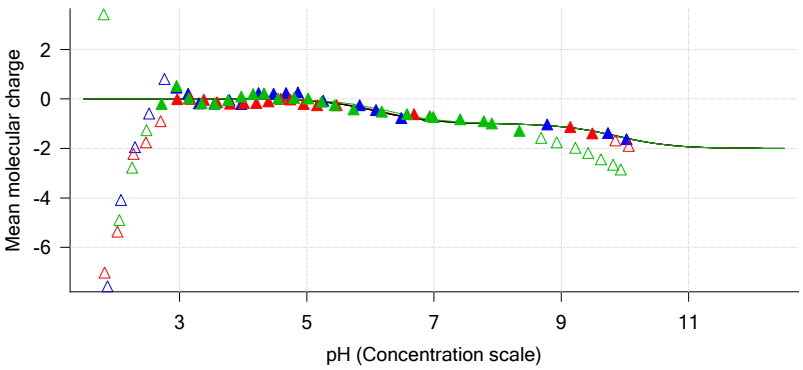
Lipophilicity Profile



Log R Profile



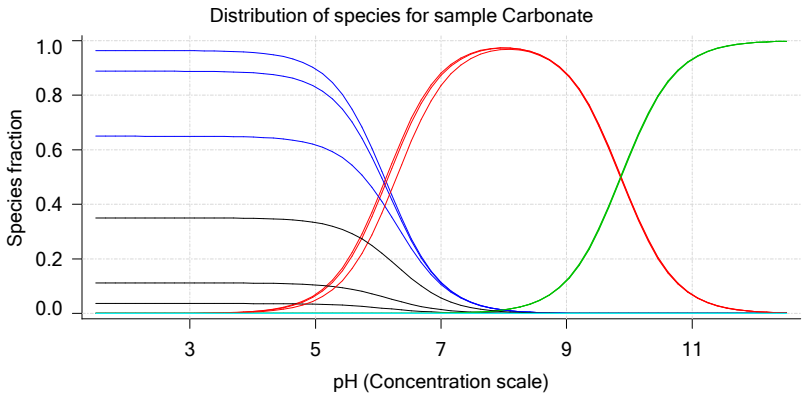
Sample Carbonate Ionisation Graph



Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)



Sample name:	**M07_octanol**	Experiment start time:	**2/28/2018 4:26:20 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18B-28011**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 1 of 3 18B-28011 Points 1 to 22

Overall results

RMSD	0.037
Average ionic strength	0.157 M
Average temperature	25.0°C
Partition ratio	0.0123 : 1
Analyte concentration range	2362.2 µM to 2434.4 µM
Total points considered	17 of 22

Warnings and errors

Errors	None
Warnings	None

Four-Plus parameters

Alpha	0.130	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r
S	0.9970	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r
jH	0.8	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r
jOH	-0.4	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r

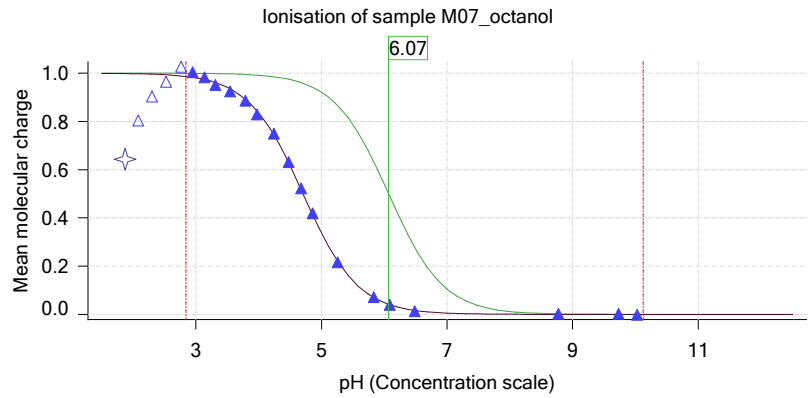
Titrants

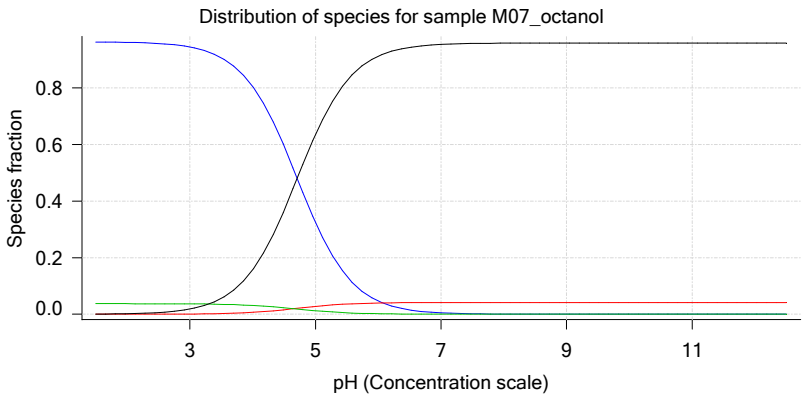
0.50 M HCl	0.993513	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH	0.999845	2/28/2018 4:26:20 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M07_octanol concentration factor	1.039
Base pKa 1	6.07
logP (XH +)	0.50
logP (neutral X)	3.27

Sample graphs

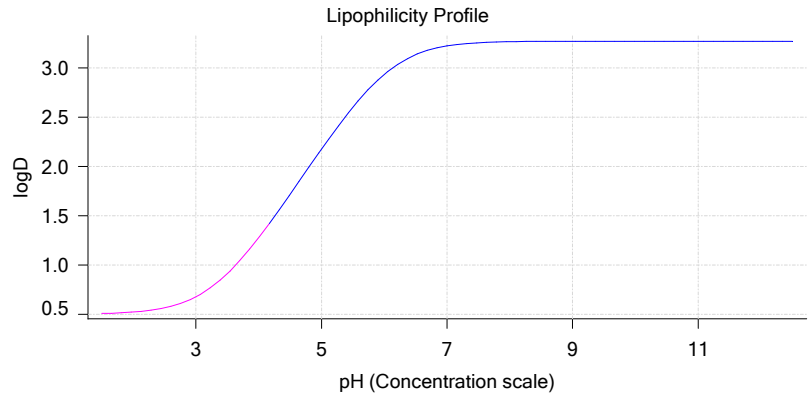




Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



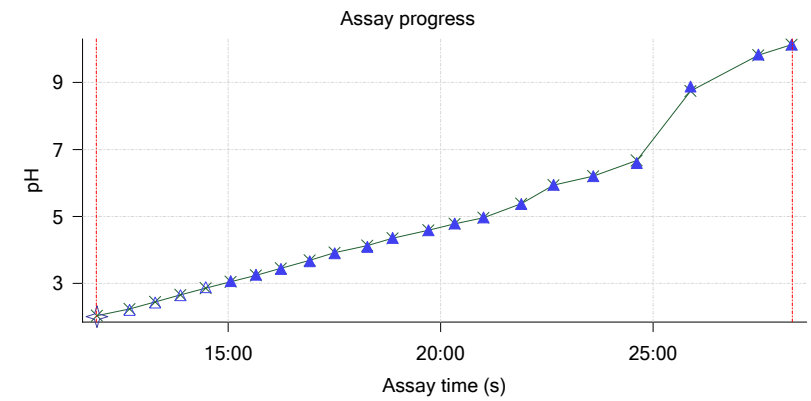
Sample logD and percent species

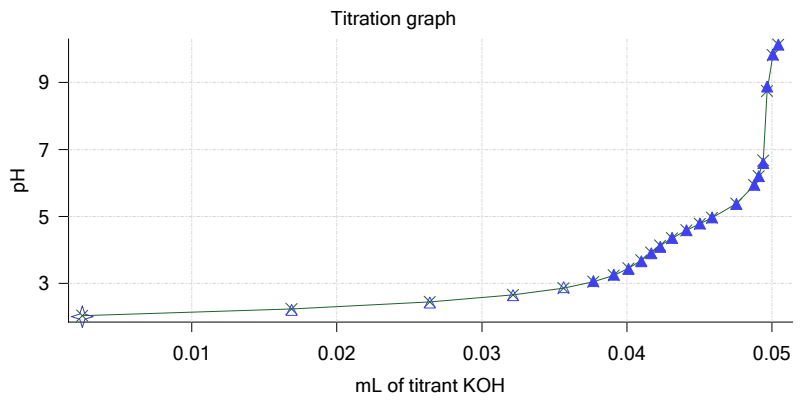
pH	M07_octanol logD	M07_octanol M07_octanolH	M07_octanol M07_octanol	M07_octanol M07_octanolH*	M07_octanol M07_octanol*	Comment
1.000	0.50	96.24 %	0.00 %	3.74 %	0.02 %	
1.200	0.50	96.23 %	0.00 %	3.74 %	0.03 %	Stomach pH
2.000	0.52	96.07 %	0.01 %	3.73 %	0.19 %	
3.000	0.68	94.41 %	0.08 %	3.67 %	1.84 %	
4.000	1.28	80.48 %	0.69 %	3.13 %	15.71 %	
5.000	2.17	32.51 %	2.77 %	1.26 %	63.46 %	
6.000	2.93	4.67 %	3.98 %	0.18 %	91.17 %	
6.500	3.13	1.53 %	4.11 %	0.06 %	94.30 %	
7.000	3.22	0.49 %	4.16 %	0.02 %	95.33 %	
7.400	3.25	0.20 %	4.17 %	0.01 %	95.63 %	Blood pH
8.000	3.27	0.05 %	4.18 %	0.00 %	95.77 %	
9.000	3.27	0.00 %	4.18 %	0.00 %	95.82 %	
10.000	3.27	0.00 %	4.18 %	0.00 %	95.82 %	
11.000	3.27	0.00 %	4.18 %	0.00 %	95.82 %	
12.000	3.27	0.00 %	4.18 %	0.00 %	95.82 %	

Carbonate and acidity

Carbonate 0.120 mM
Acidity error 0.213 mM

Other graphs

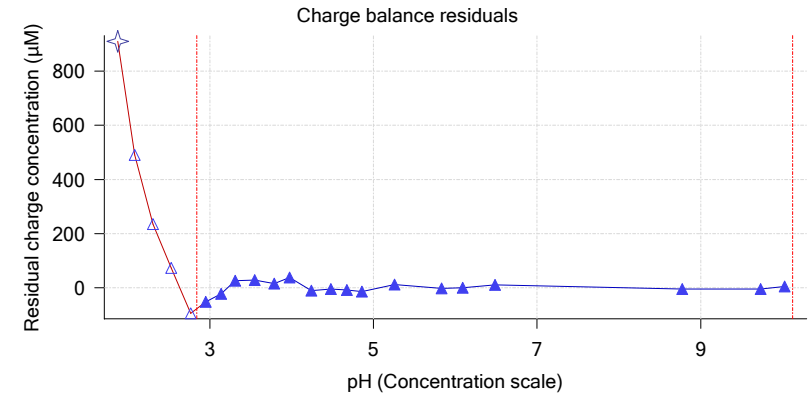


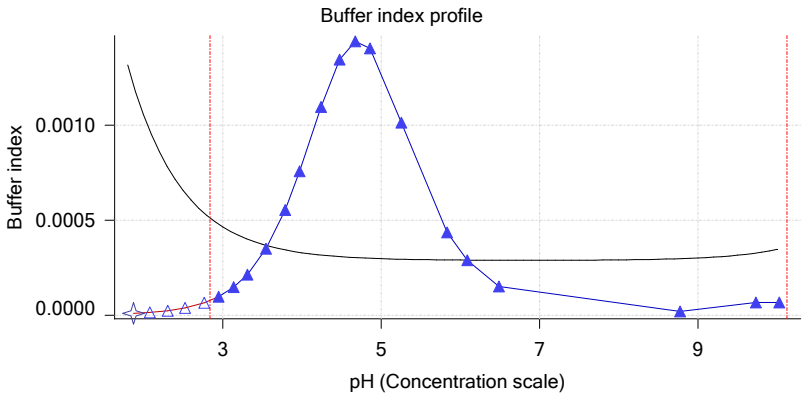


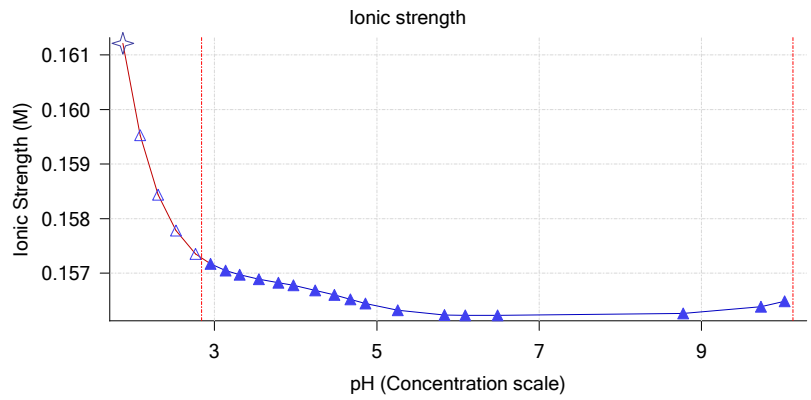
Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

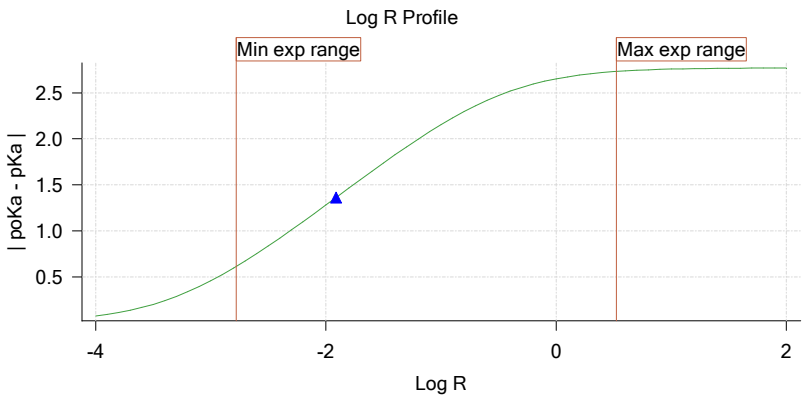
Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

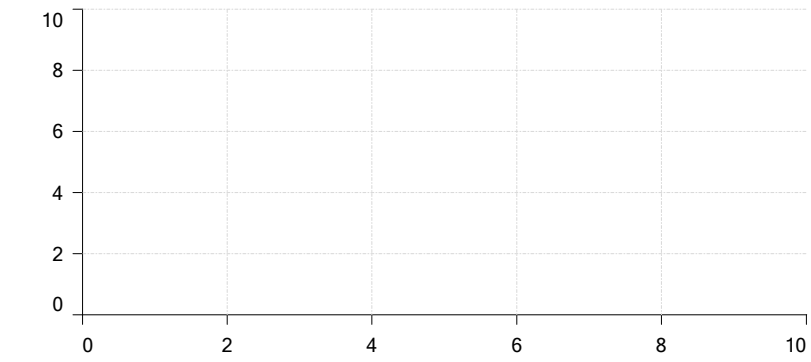
Other graphs (continued)

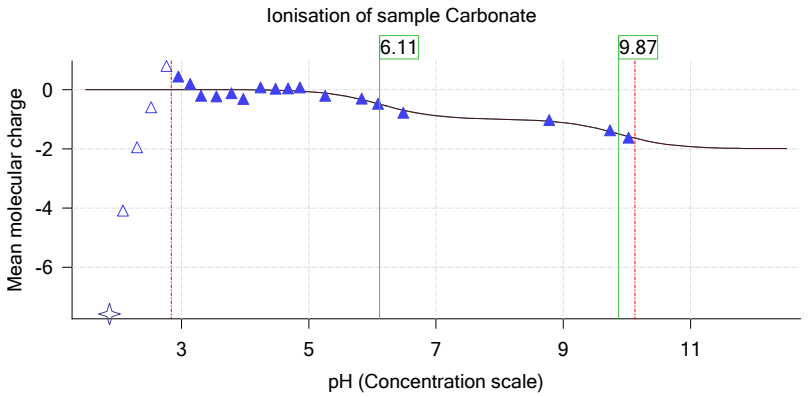












Sample name:	**M07_octanol**	Experiment start time:	**2/28/2018 4:26:20 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18B-28011**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 2 of 3 18B-28011 Points 23 to 45

Overall results

RMSD	0.084
Average ionic strength	0.162 M
Average temperature	25.0°C
Partition ratio	0.0408 : 1
Analyte concentration range	2150.3 µM to 2218.8 µM
Total points considered	16 of 23

Warnings and errors

Errors	None
Warnings	None

Four-Plus parameters

Alpha	0.130	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r
S	0.9970	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r
jH	0.8	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r
jOH	-0.4	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r

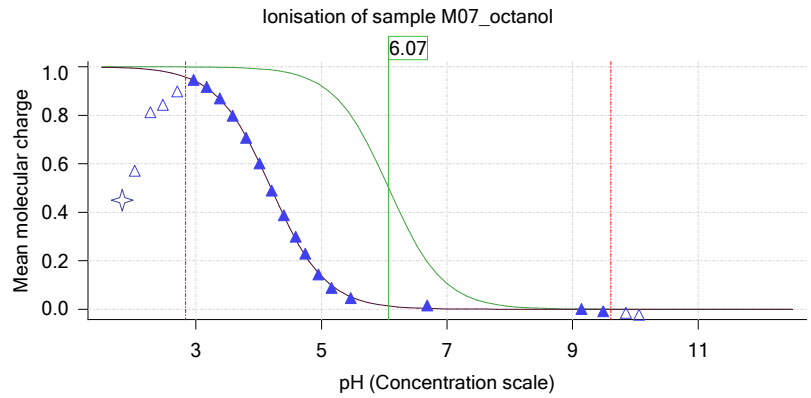
Titrants

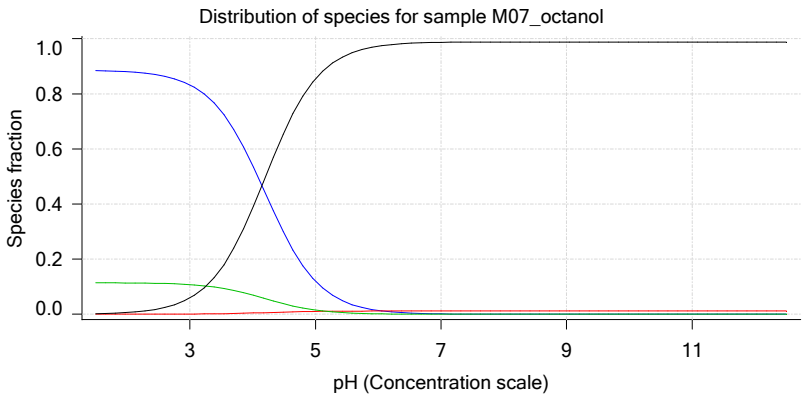
0.50 M HCl	0.993513	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH	0.999845	2/28/2018 4:26:20 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M07_octanol concentration factor	1.041
Base pKa 1	6.07
logP (XH +)	0.50
logP (neutral X)	3.31

Sample graphs

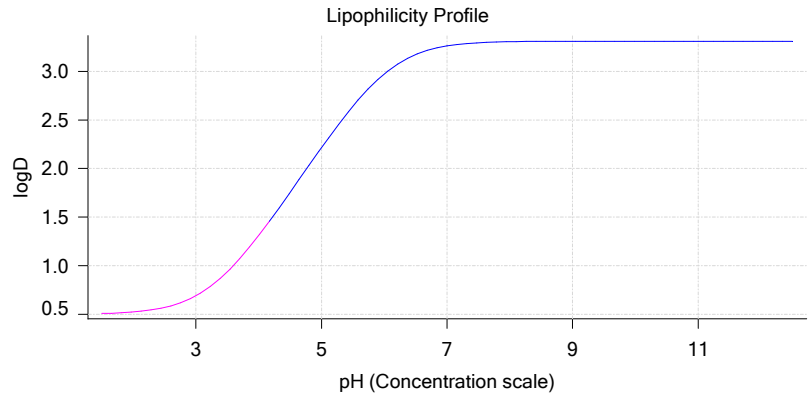




Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



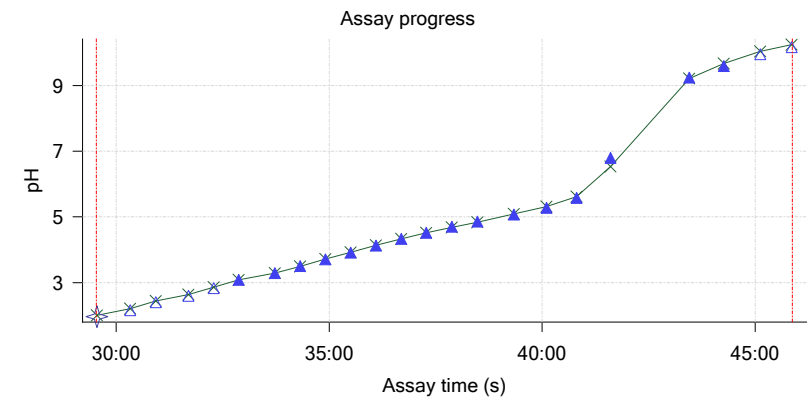
Sample logD and percent species

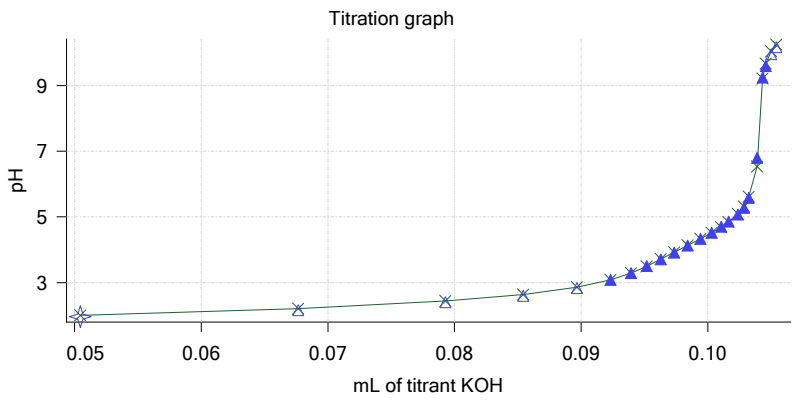
pH	M07_octanol logD	M07_octanol M07_octanolH	M07_octanol M07_octanol	M07_octanol M07_octanolH*	M07_octanol M07_octanol*	Comment
1.000	0.50	88.51 %	0.00 %	11.43 %	0.06 %	
1.200	0.50	88.48 %	0.00 %	11.42 %	0.10 %	Stomach pH
2.000	0.52	88.01 %	0.01 %	11.36 %	0.63 %	
3.000	0.69	83.26 %	0.07 %	10.75 %	5.92 %	
4.000	1.31	54.08 %	0.46 %	6.98 %	38.48 %	
5.000	2.21	12.01 %	1.02 %	1.55 %	85.42 %	
6.000	2.97	1.37 %	1.16 %	0.18 %	97.29 %	
6.500	3.17	0.44 %	1.18 %	0.06 %	98.33 %	
7.000	3.26	0.14 %	1.18 %	0.02 %	98.66 %	
7.400	3.29	0.06 %	1.18 %	0.01 %	98.76 %	Blood pH
8.000	3.31	0.01 %	1.18 %	0.00 %	98.80 %	
9.000	3.31	0.00 %	1.18 %	0.00 %	98.82 %	
10.000	3.31	0.00 %	1.18 %	0.00 %	98.82 %	
11.000	3.31	0.00 %	1.18 %	0.00 %	98.82 %	
12.000	3.31	0.00 %	1.18 %	0.00 %	98.82 %	

Carbonate and acidity

Carbonate 0.188 mM
Acidity error 0.195 mM

Other graphs

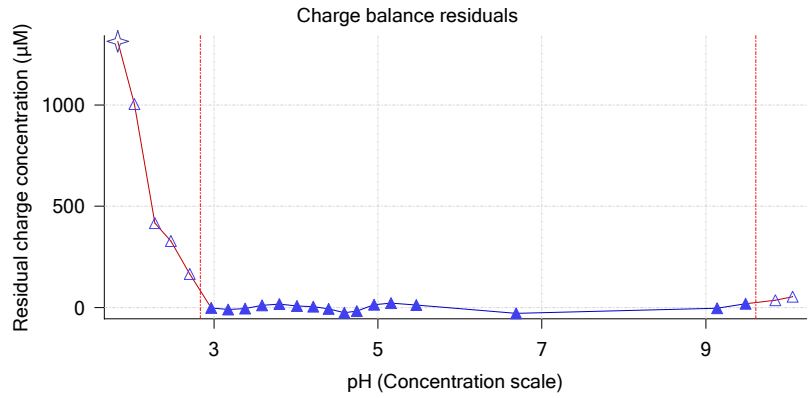


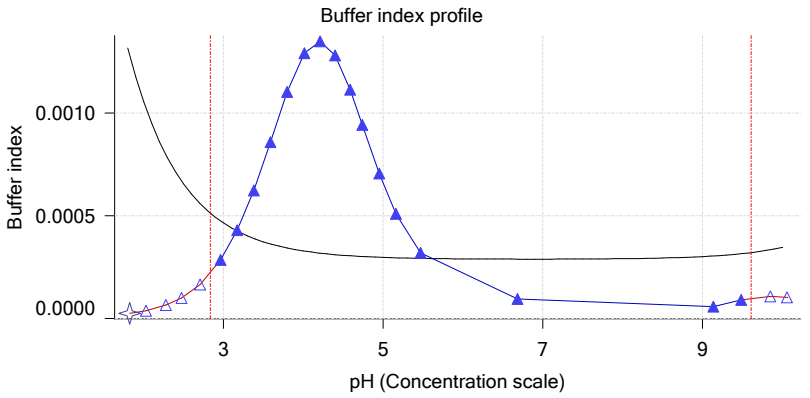


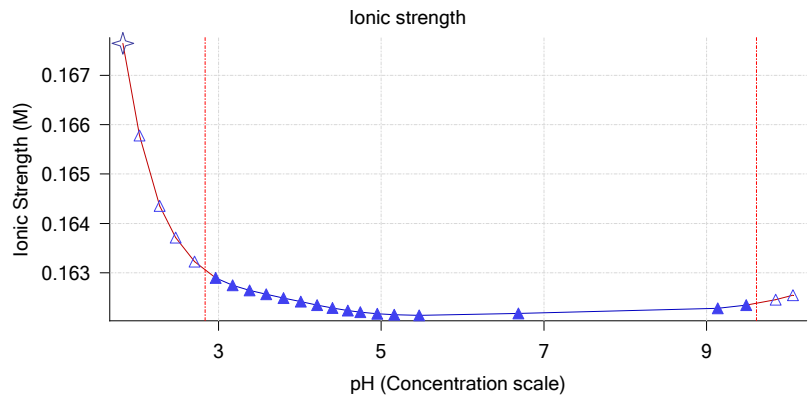
Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

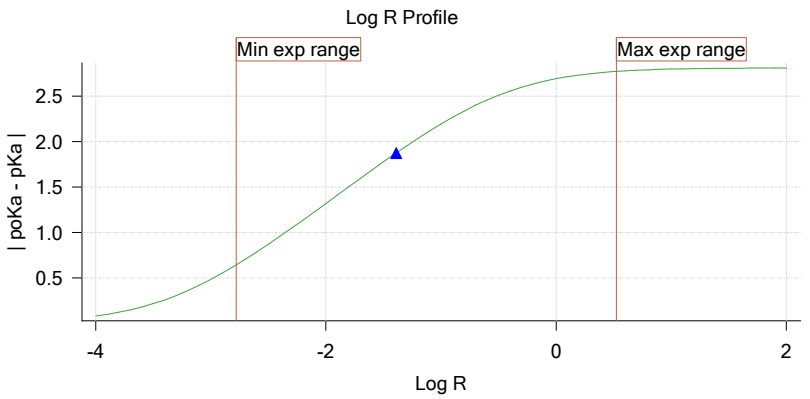
Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

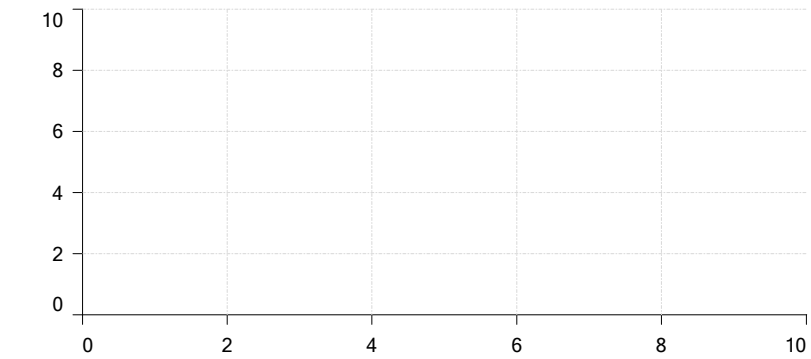
Other graphs (continued)

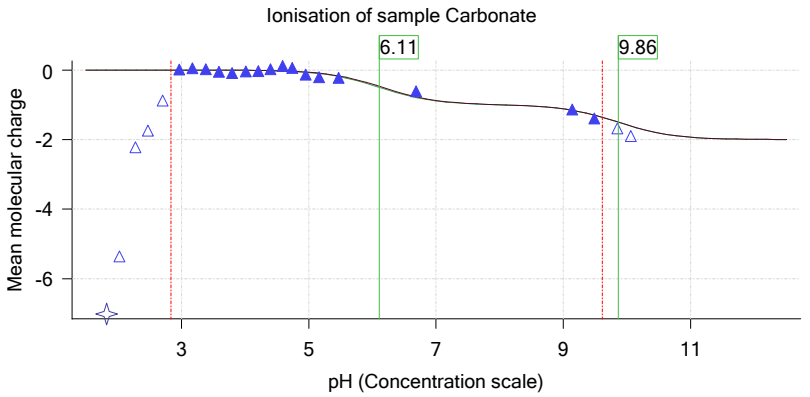












Sample name:	**M07_octanol**	Experiment start time:	**2/28/2018 4:26:20 PM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18B-28011**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 3 of 3 18B-28011 Points 46 to 79

Overall results

RMSD	0.443
Average ionic strength	0.169 M
Average temperature	25.0°C
Partition ratio	0.1746 : 1
Analyte concentration range	1775.6 µM to 1831.9 µM
Total points considered	23 of 34

Warnings and errors

Errors	None
Warnings	Excessive acidity error present

Four-Plus parameters

Alpha	0.130	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r
S	0.9970	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r
jH	0.8	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r
jOH	-0.4	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r

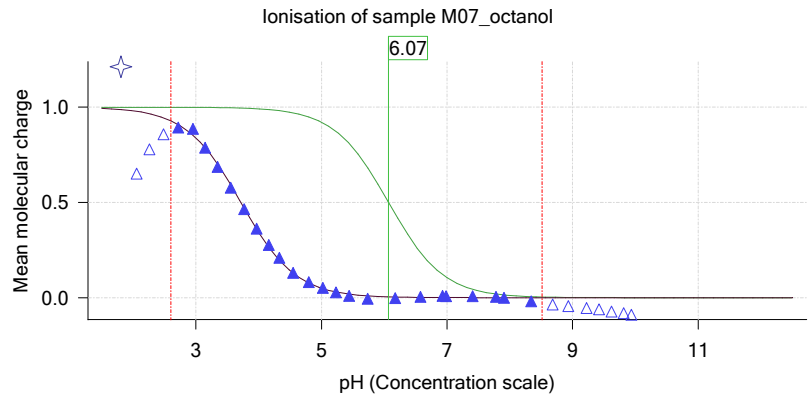
Titrants

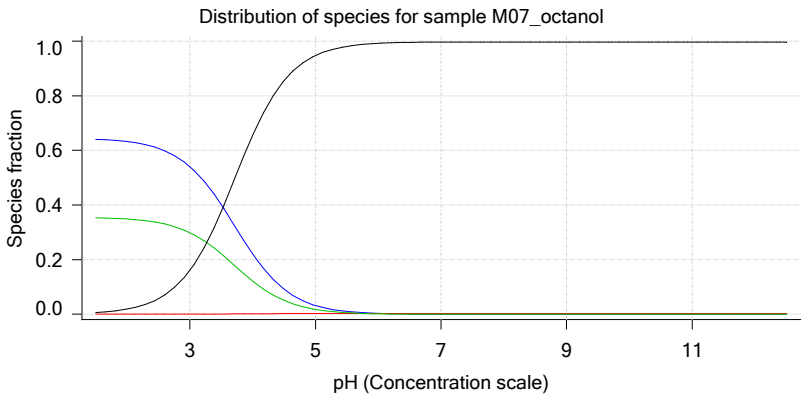
0.50 M HCl	0.993513	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH	0.999845	2/28/2018 4:26:20 PM	C:\Sirius_T3\KOH18B27.t3r

Sample

M07_octanol concentration factor	0.988
Base pKa 1	6.07
logP (XH +)	0.50
logP (neutral X)	3.30

Sample graphs

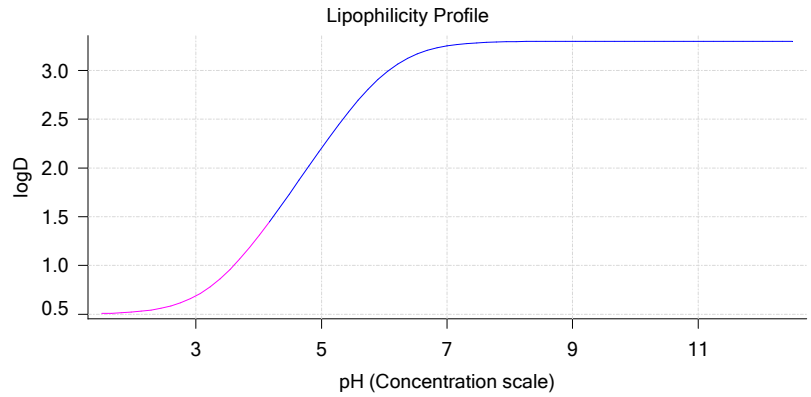




Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



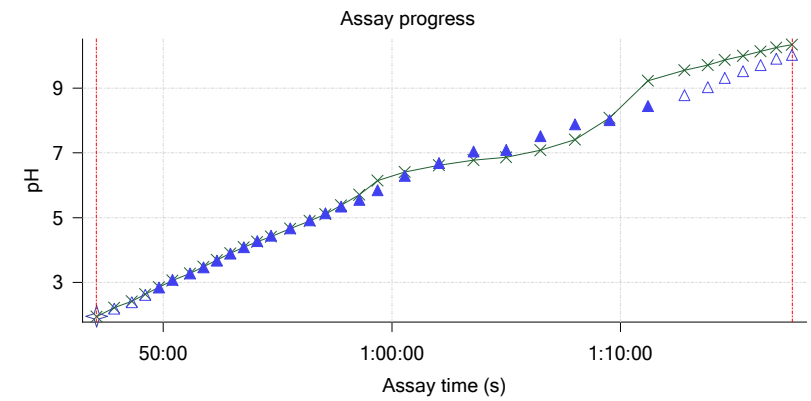
Sample logD and percent species

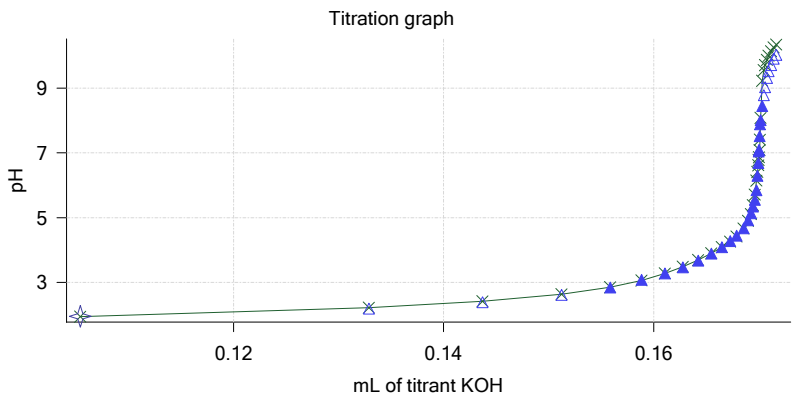
pH	M07_octanol logD	M07_octanol M07_octanolH	M07_octanol M07_octanol	M07_octanol M07_octanolH*	M07_octanol M07_octanol*	Comment
1.000	0.50	64.31 %	0.00 %	35.50 %	0.19 %	
1.200	0.50	64.24 %	0.00 %	35.46 %	0.30 %	Stomach pH
2.000	0.52	63.22 %	0.01 %	34.90 %	1.88 %	
3.000	0.69	54.07 %	0.05 %	29.85 %	16.04 %	
4.000	1.30	22.09 %	0.19 %	12.19 %	65.53 %	
5.000	2.20	3.20 %	0.27 %	1.76 %	94.77 %	
6.000	2.96	0.33 %	0.28 %	0.18 %	99.20 %	
6.500	3.16	0.11 %	0.29 %	0.06 %	99.55 %	
7.000	3.25	0.03 %	0.29 %	0.02 %	99.66 %	
7.400	3.28	0.01 %	0.29 %	0.01 %	99.69 %	Blood pH
8.000	3.30	0.00 %	0.29 %	0.00 %	99.71 %	
9.000	3.30	0.00 %	0.29 %	0.00 %	99.71 %	
10.000	3.30	0.00 %	0.29 %	0.00 %	99.71 %	
11.000	3.30	0.00 %	0.29 %	0.00 %	99.71 %	
12.000	3.30	0.00 %	0.29 %	0.00 %	99.71 %	

Carbonate and acidity

Carbonate 0.141 mM
Acidity error 2.186 mM

Other graphs

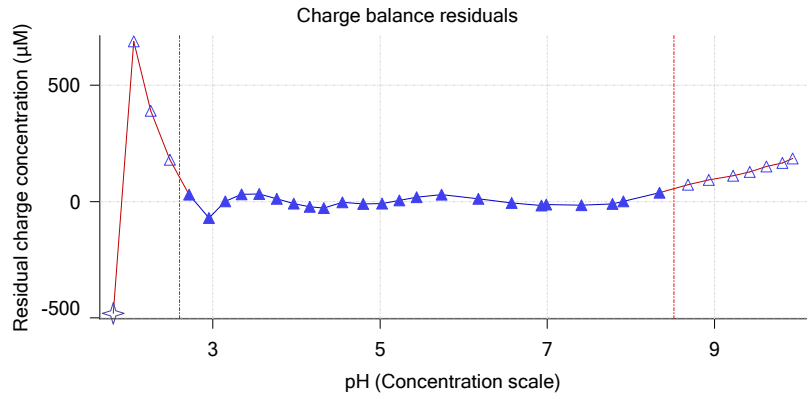


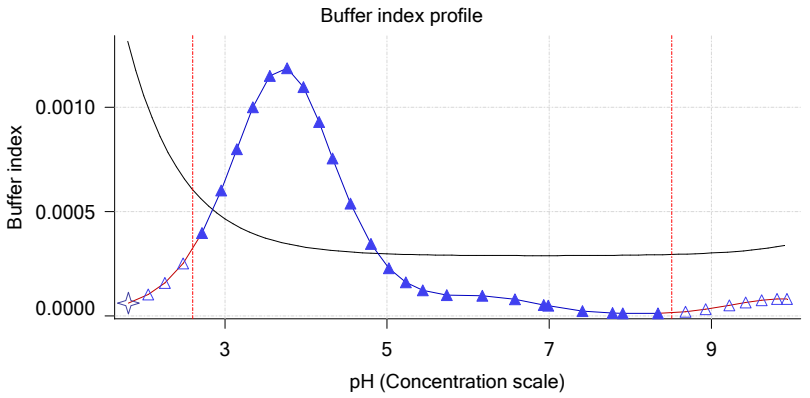


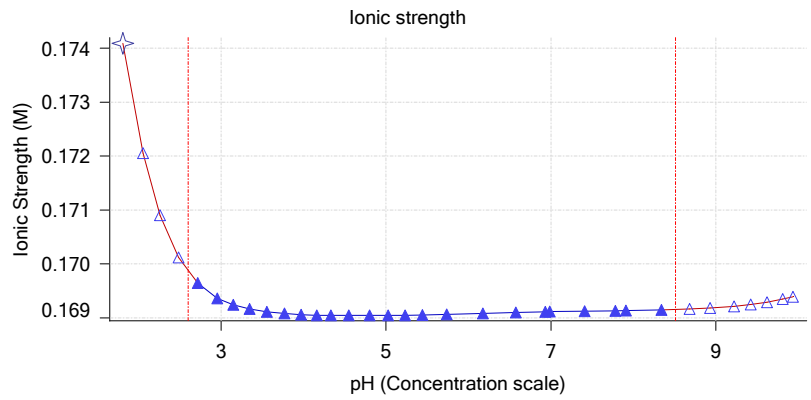
Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

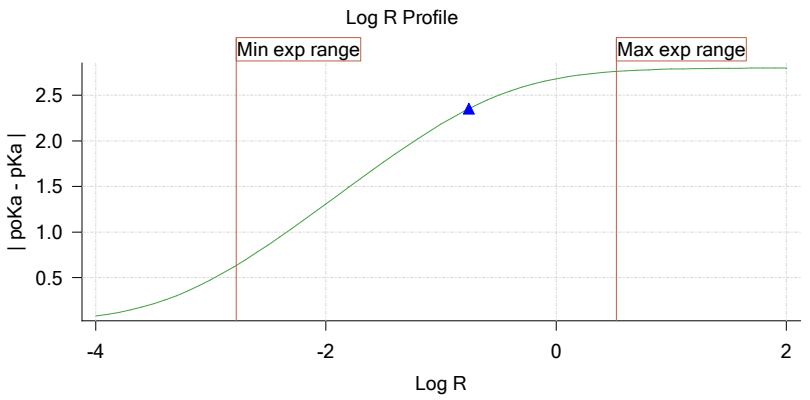
Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

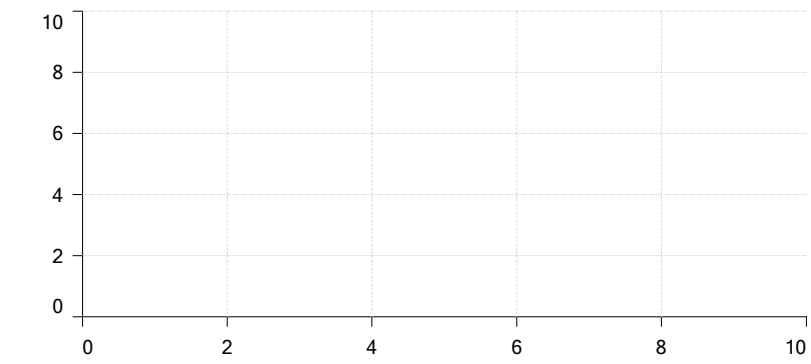
Other graphs (continued)

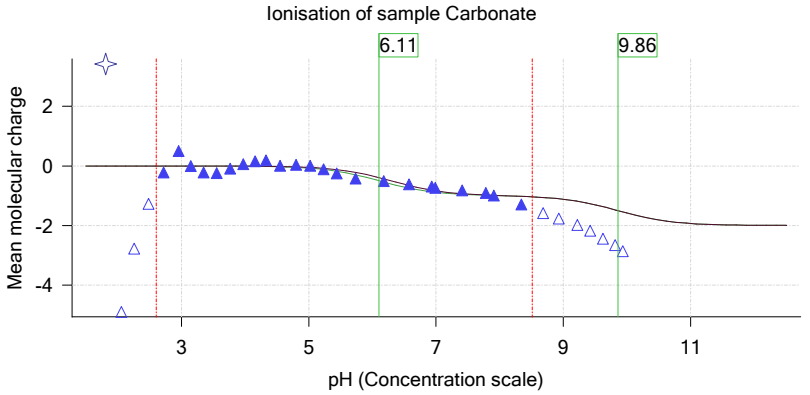












Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M07_octanol	2/27/2018 4:29:24 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.000900 g	2/28/2018 4:24:06 PM	User entered value
Formula weight	235.28 g/mol	2/27/2018 4:29:24 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	235.28	2/27/2018 4:29:24 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	1	2/27/2018 4:29:24 PM	User entered value
Sample is a	Base	2/27/2018 4:29:24 PM	User entered value
pKa 1	6.07	2/27/2018 4:29:24 PM	User entered value
logp (XH +)	0.50	2/28/2018 1:33:04 PM	User entered value
logP (neutral X)	3.44	2/28/2018 1:33:10 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
8:55.6	Initial pH = 6.32									
11:55.1	Data point 1	1.50000 mL	0.04887 mL	0.00245 mL	0.01999 mL	2.007	-0.00759	0.43163	0.00057	10.0 s
12:41.2	Data point 2	1.50000 mL	0.04887 mL	0.01689 mL	0.01999 mL	2.212	-0.00650	0.83933	0.00035	10.5 s
13:17.4	Data point 3	1.50000 mL	0.04887 mL	0.02641 mL	0.01999 mL	2.431	-0.00986	0.77807	0.00055	10.0 s
13:52.9	Data point 4	1.50000 mL	0.04887 mL	0.03215 mL	0.01999 mL	2.651	-0.00451	0.66680	0.00027	10.0 s
14:28.4	Data point 5	1.50000 mL	0.04887 mL	0.03563 mL	0.01999 mL	2.888	-0.00773	0.36187	0.00063	10.0 s
15:03.8	Data point 6	1.50000 mL	0.04887 mL	0.03770 mL	0.01999 mL	3.072	-0.00302	0.21499	0.00032	10.0 s
15:39.3	Data point 7	1.50000 mL	0.04887 mL	0.03911 mL	0.01999 mL	3.259	-0.00406	0.30171	0.00036	10.0 s
16:14.6	Data point 8	1.50000 mL	0.04887 mL	0.04012 mL	0.01999 mL	3.431	-0.00336	0.75731	0.00019	10.0 s
16:55.2	Data point 9	1.50000 mL	0.04887 mL	0.04099 mL	0.01999 mL	3.667	-0.00529	0.80865	0.00029	10.0 s
17:30.5	Data point 10	1.50000 mL	0.04887 mL	0.04167 mL	0.01999 mL	3.906	-0.01649	0.89884	0.00086	10.5 s
18:16.6	Data point 11	1.50000 mL	0.04887 mL	0.04231 mL	0.01999 mL	4.090	-0.00742	0.86888	0.00039	10.0 s
18:52.0	Data point 12	1.50000 mL	0.04887 mL	0.04311 mL	0.01999 mL	4.359	-0.01526	0.79653	0.00084	10.0 s
19:43.0	Data point 13	1.50000 mL	0.04887 mL	0.04412 mL	0.01999 mL	4.593	-0.01458	0.78492	0.00081	11.5 s
20:19.9	Data point 14	1.50000 mL	0.04887 mL	0.04504 mL	0.01999 mL	4.792	-0.01834	0.83155	0.00099	15.0 s
21:00.3	Data point 15	1.50000 mL	0.04887 mL	0.04588 mL	0.01999 mL	4.975	-0.01816	0.89144	0.00095	12.5 s
21:53.9	Data point 16	1.50000 mL	0.04887 mL	0.04755 mL	0.01999 mL	5.371	-0.01774	0.89163	0.00093	15.0 s
22:39.5	Data point 17	1.50000 mL	0.04887 mL	0.04880 mL	0.01999 mL	5.944	-0.01937	0.91808	0.00100	25.5 s
23:35.6	Data point 18	1.50000 mL	0.04887 mL	0.04911 mL	0.01999 mL	6.201	-0.01860	0.87008	0.00098	25.5 s
24:36.8	Data point 19	1.50000 mL	0.04887 mL	0.04941 mL	0.01999 mL	6.598	-0.01882	0.95235	0.00095	40.0 s
25:52.5	Data point 20	1.50000 mL	0.04887 mL	0.04967 mL	0.01999 mL	8.879	-0.02286	0.13576	0.00307	Timed out at 59.5 s
27:28.2	Data point 21	1.50000 mL	0.04887 mL	0.05007 mL	0.01999 mL	9.833	-0.01571	0.67713	0.00094	16.5 s
28:15.3	Data point 22	1.50000 mL	0.04887 mL	0.05045 mL	0.01999 mL	10.125	-0.01833	0.90348	0.00095	18.5 s
29:33.1	Data point 23	1.50000 mL	0.10350 mL	0.05045 mL	0.06999 mL	1.961	-0.00524	0.41258	0.00040	10.5 s
30:19.8	Data point 24	1.50000 mL	0.10350 mL	0.06766 mL	0.06999 mL	2.160	-0.01414	0.83789	0.00076	10.5 s
30:56.0	Data point 25	1.50000 mL	0.10350 mL	0.07928 mL	0.06999 mL	2.405	0.00314	0.09186	0.00051	10.0 s
31:42.0	Data point 26	1.50000 mL	0.10350 mL	0.08542 mL	0.06999 mL	2.598	-0.00349	0.57578	0.00023	10.0 s
32:17.4	Data point 27	1.50000 mL	0.10350 mL	0.08968 mL	0.06999 mL	2.829	-0.00230	0.56610	0.00015	10.0 s
32:52.8	Data point 28	1.50000 mL	0.10350 mL	0.09231 mL	0.06999 mL	3.088	-0.00226	0.48854	0.00016	10.0 s
33:43.8	Data point 29	1.50000 mL	0.10350 mL	0.09393 mL	0.06999 mL	3.295	0.00205	0.02071	0.00070	10.0 s
34:19.2	Data point 30	1.50000 mL	0.10350 mL	0.09518 mL	0.06999 mL	3.501	-0.00570	0.60687	0.00036	10.0 s
34:54.6	Data point 31	1.50000 mL	0.10350 mL	0.09628 mL	0.06999 mL	3.707	-0.00228	0.44952	0.00017	10.5 s
35:30.6	Data point 32	1.50000 mL	0.10350 mL	0.09734 mL	0.06999 mL	3.917	-0.00812	0.27411	0.00077	10.0 s
36:06.0	Data point 33	1.50000 mL	0.10350 mL	0.09840 mL	0.06999 mL	4.130	-0.00941	0.30499	0.00084	10.0 s
36:41.4	Data point 34	1.50000 mL	0.10350 mL	0.09941 mL	0.06999 mL	4.327	0.00167	0.00821	0.00091	10.0 s
37:16.9	Data point 35	1.50000 mL	0.10350 mL	0.10031 mL	0.06999 mL	4.517	-0.00558	0.51690	0.00038	10.5 s
37:52.8	Data point 36	1.50000 mL	0.10350 mL	0.10106 mL	0.06999 mL	4.705	-0.00463	0.40740	0.00036	10.5 s
38:28.8	Data point 37	1.50000 mL	0.10350 mL	0.10165 mL	0.06999 mL	4.857	-0.00336	0.10816	0.00050	10.5 s
39:20.2	Data point 38	1.50000 mL	0.10350 mL	0.10237 mL	0.06999 mL	5.067	-0.00648	0.11307	0.00095	10.5 s
40:06.4	Data point 39	1.50000 mL	0.10350 mL	0.10285 mL	0.06999 mL	5.275	0.00498	0.07222	0.00091	11.5 s

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
40:48.5	Data point 40	1.50000 mL	0.10350 mL	0.10325 mL	0.06999 mL	5.581	-0.01086	0.46682	0.00078	12.0 s
41:36.2	Data point 41	1.50000 mL	0.10350 mL	0.10388 mL	0.06999 mL	6.795	-0.04882	0.99621	0.00241	Timed out at 59.5 s
43:27.1	Data point 42	1.50000 mL	0.10350 mL	0.10433 mL	0.06999 mL	9.241	-0.00847	0.26017	0.00082	18.5 s
44:16.0	Data point 43	1.50000 mL	0.10350 mL	0.10459 mL	0.06999 mL	9.587	-0.01617	0.74261	0.00093	21.0 s
45:07.4	Data point 44	1.50000 mL	0.10350 mL	0.10501 mL	0.06999 mL	9.949	-0.01841	0.93681	0.00094	13.5 s
45:51.4	Data point 45	1.50000 mL	0.10350 mL	0.10541 mL	0.06999 mL	10.160	-0.00819	0.56417	0.00054	10.0 s
47:05.4	Data point 46	1.50000 mL	0.16268 mL	0.10541 mL	0.31999 mL	1.946	-0.00597	0.52848	0.00041	10.0 s
47:51.7	Data point 47	1.50000 mL	0.16268 mL	0.13290 mL	0.31999 mL	2.185	0.00614	0.38583	0.00049	10.0 s
48:37.7	Data point 48	1.50000 mL	0.16268 mL	0.14372 mL	0.31999 mL	2.386	-0.00203	0.41833	0.00016	10.0 s
49:13.2	Data point 49	1.50000 mL	0.16268 mL	0.15122 mL	0.31999 mL	2.611	0.01311	0.84025	0.00071	10.0 s
49:48.7	Data point 50	1.50000 mL	0.16268 mL	0.15588 mL	0.31999 mL	2.842	0.00403	0.34986	0.00034	10.0 s
50:24.2	Data point 51	1.50000 mL	0.16268 mL	0.15887 mL	0.31999 mL	3.077	-0.00378	0.75203	0.00022	10.0 s
51:10.1	Data point 52	1.50000 mL	0.16268 mL	0.16108 mL	0.31999 mL	3.269	0.00384	0.15940	0.00048	10.0 s
51:45.5	Data point 53	1.50000 mL	0.16268 mL	0.16279 mL	0.31999 mL	3.466	-0.00301	0.05747	0.00062	10.0 s
52:20.9	Data point 54	1.50000 mL	0.16268 mL	0.16425 mL	0.31999 mL	3.673	0.00201	0.08022	0.00035	10.0 s
52:56.4	Data point 55	1.50000 mL	0.16268 mL	0.16550 mL	0.31999 mL	3.886	-0.00573	0.82166	0.00031	10.0 s
53:31.7	Data point 56	1.50000 mL	0.16268 mL	0.16651 mL	0.31999 mL	4.087	-0.00755	0.87150	0.00040	10.0 s
54:07.0	Data point 57	1.50000 mL	0.16268 mL	0.16731 mL	0.31999 mL	4.277	-0.00644	0.13717	0.00086	10.0 s
54:42.4	Data point 58	1.50000 mL	0.16268 mL	0.16790 mL	0.31999 mL	4.446	-0.01161	0.50856	0.00080	10.0 s
55:33.2	Data point 59	1.50000 mL	0.16268 mL	0.16858 mL	0.31999 mL	4.665	-0.00119	0.00535	0.00080	10.5 s
56:24.4	Data point 60	1.50000 mL	0.16268 mL	0.16900 mL	0.31999 mL	4.916	-0.00586	0.09627	0.00093	10.5 s
57:05.5	Data point 61	1.50000 mL	0.16268 mL	0.16926 mL	0.31999 mL	5.139	0.00326	0.04495	0.00076	11.0 s
57:47.1	Data point 62	1.50000 mL	0.16268 mL	0.16947 mL	0.31999 mL	5.345	-0.00065	0.00209	0.00070	11.5 s
58:34.2	Data point 63	1.50000 mL	0.16268 mL	0.16964 mL	0.31999 mL	5.553	0.00764	0.15851	0.00095	12.5 s
59:22.4	Data point 64	1.50000 mL	0.16268 mL	0.16980 mL	0.31999 mL	5.848	-0.01710	0.92021	0.00088	35.5 s
1:00:33.7	Data point 65	1.50000 mL	0.16268 mL	0.16990 mL	0.31999 mL	6.288	-0.01881	0.94810	0.00095	59.5 s
1:02:03.8	Data point 66	1.50000 mL	0.16268 mL	0.16997 mL	0.31999 mL	6.686	-0.05982	0.98248	0.00298	Timed out at 59.5 s
1:03:34.3	Data point 67	1.50000 mL	0.16268 mL	0.17001 mL	0.31999 mL	7.040	-0.07343	0.98170	0.00366	Timed out at 59.5 s
1:04:59.6	Data point 68	1.50000 mL	0.16268 mL	0.17004 mL	0.31999 mL	7.096	-0.04310	0.98785	0.00214	Timed out at 59.5 s
1:06:30.2	Data point 69	1.50000 mL	0.16268 mL	0.17008 mL	0.31999 mL	7.517	-0.07608	0.99474	0.00377	Timed out at 59.5 s
1:08:00.6	Data point 70	1.50000 mL	0.16268 mL	0.17013 mL	0.31999 mL	7.886	-0.06164	0.99333	0.00306	Timed out at 59.5 s
1:09:31.1	Data point 71	1.50000 mL	0.16268 mL	0.17018 mL	0.31999 mL	8.015	-0.04517	0.98471	0.00225	Timed out at 59.5 s
1:11:11.9	Data point 72	1.50000 mL	0.16268 mL	0.17034 mL	0.31999 mL	8.445	-0.02344	0.95432	0.00119	Timed out at 59.5 s
1:12:47.5	Data point 73	1.50000 mL	0.16268 mL	0.17051 mL	0.31999 mL	8.787	-0.01486	0.61766	0.00093	20.5 s
1:13:48.8	Data point 74	1.50000 mL	0.16268 mL	0.17063 mL	0.31999 mL	9.033	-0.01484	0.60375	0.00094	13.5 s
1:14:33.0	Data point 75	1.50000 mL	0.16268 mL	0.17079 mL	0.31999 mL	9.324	-0.01384	0.49067	0.00098	17.5 s
1:15:21.1	Data point 76	1.50000 mL	0.16268 mL	0.17096 mL	0.31999 mL	9.524	-0.01653	0.72433	0.00096	10.5 s
1:16:07.3	Data point 77	1.50000 mL	0.16268 mL	0.17119 mL	0.31999 mL	9.720	-0.01049	0.45814	0.00077	10.5 s
1:16:48.4	Data point 78	1.50000 mL	0.16268 mL	0.17145 mL	0.31999 mL	9.913	-0.00202	0.02625	0.00062	10.5 s
1:17:29.5	Data point 79	1.50000 mL	0.16268 mL	0.17168 mL	0.31999 mL	10.034	-0.01309	0.45959	0.00095	13.0 s
1:17:51.5	Assay volumes	1.50000 mL	0.16268 mL	0.17168 mL	0.31999 mL					

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	10.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	1.50 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.020 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	300 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.050 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**
Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.250 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.130	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus S	0.9970	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jH	0.8	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jOH	-0.4	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r
Base concentration factor	1.000	2/28/2018 4:26:20 PM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.994	2/28/2018 4:26:20 PM	C:\Sirius_T3\HCl18B27.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	2/28/2018 10:18:04 AM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+3.96 mV		2/28/2018 4:27:04 PM
Filling solution	3M KCl	KCL097	2/27/2018 9:49:43 AM
Liquids			
Wash 1	50% IPA:50% Water		2/28/2018 10:23:32 AM
Wash 2	0.5% Trition X-100 in H20		2/28/2018 10:23:34 AM
Buffer position 1	pH7 Wash		2/28/2018 10:24:06 AM
Buffer position 2	pH 7		2/28/2018 10:24:08 AM
Storage position			2/28/2018 10:21:14 AM
Wash water	8.8e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	6.7e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	112:08:55		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[1:57] Air gap released for Acid (0.5 M HCl)
[1:57] Air gap released for Base (0.5 M KOH)
[2:33] Air gap created for Water (0.15 M KCl)
[2:33] Air gap created for Acid (0.5 M HCl)
[2:33] Air gap created for Base (0.5 M KOH)
[2:34] Air gap released for Water (0.15 M KCl)
[2:38] Titrator arm moved over Titration position
[2:38] Titration 1 of 3
[2:38] Adding initial titrants
[2:38] Automatically add 1.50000 mL of water
[3:03] Dispensed 1.500000 mL of Water (0.15 M KCl)
[3:07] Titrator arm moved over Drain
[8:49] Titrator arm moved to Titration position
[8:49] Argon flow rate set to 100
[8:49] Stirrer speed set to 10
[8:54] Automatically add 0.02000 mL of Octanol
[8:54] Dispensed 0.019991 mL of Octanol
[8:55] Initial pH = 6.32
[8:55] Iterative adjust 6.32 -> 2.00
[8:55] pH 6.32 -> 2.00
[8:57] Air gap released for Acid (0.5 M HCl)
[8:58] Dispensed 0.048871 mL of Acid (0.5 M HCl)
[9:03] Holding pH 2.00
[11:03] Stirrer speed set to 0
[11:03] Stirrer speed set to 50
[11:03] Iterative adjust 1.98 -> 2.00
[11:03] pH 1.98 -> 2.00
[11:04] Air gap released for Base (0.5 M KOH)
[11:04] Dispensed 0.002446 mL of Base (0.5 M KOH)
[11:55] Stirrer speed set to 0
[12:05] Datapoint id 1 collected
[12:05] Stirrer speed set to 50
[12:10] pH 2.02 -> 2.22
[12:10] Using cautious pH adjust
[12:10] Dispensed 0.007643 mL of Base (0.5 M KOH)
[12:15] Stepping pH = 2.11
[12:16] Dispensed 0.005339 mL of Base (0.5 M KOH)
[12:21] Stepping pH = 2.19
[12:21] Dispensed 0.001458 mL of Base (0.5 M KOH)
[12:26] Stepping pH = 2.22
[12:41] Stirrer speed set to 0
[12:52] Datapoint id 2 collected

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[12:52] Charge balance equation is out by 5.5%
[12:52] Stirrer speed set to 50
[12:57] pH 2.22 -> 2.42
[12:57] Using charge balance adjust
[12:57] Dispensed 0.009525 mL of Base (0.5 M KOH)
[13:17] Stirrer speed set to 0
[13:27] Datapoint id 3 collected
[13:27] Charge balance equation is out by 6.0%
[13:27] Stirrer speed set to 50
[13:32] pH 2.44 -> 2.64
[13:32] Using charge balance adjust
[13:32] Dispensed 0.005738 mL of Base (0.5 M KOH)
[13:53] Stirrer speed set to 0
[14:03] Datapoint id 4 collected
[14:03] Charge balance equation is out by 5.9%
[14:03] Stirrer speed set to 50
[14:08] pH 2.66 -> 2.86
[14:08] Using charge balance adjust
[14:08] Dispensed 0.003481 mL of Base (0.5 M KOH)
[14:28] Stirrer speed set to 0
[14:38] Datapoint id 5 collected
[14:38] Charge balance equation is out by 14.5%
[14:38] Stirrer speed set to 50
[14:43] pH 2.89 -> 3.09
[14:43] Using charge balance adjust
[14:43] Dispensed 0.002070 mL of Base (0.5 M KOH)
[15:04] Stirrer speed set to 0
[15:14] Datapoint id 6 collected
[15:14] Charge balance equation is out by -10.8%
[15:14] Stirrer speed set to 50
[15:19] pH 3.08 -> 3.28
[15:19] Using charge balance adjust
[15:19] Dispensed 0.001411 mL of Base (0.5 M KOH)
[15:39] Stirrer speed set to 0
[15:49] Datapoint id 7 collected
[15:49] Charge balance equation is out by -9.7%
[15:49] Stirrer speed set to 50
[15:54] pH 3.26 -> 3.46
[15:54] Using charge balance adjust
[15:54] Dispensed 0.001011 mL of Base (0.5 M KOH)
[16:14] Stirrer speed set to 0
[16:24] Datapoint id 8 collected
[16:24] Charge balance equation is out by -16.8%
[16:24] Stirrer speed set to 50
[16:29] pH 3.44 -> 3.64
[16:29] Using cautious pH adjust
[16:30] Dispensed 0.000400 mL of Base (0.5 M KOH)
[16:35] Stepping pH = 3.50
[16:35] Dispensed 0.000470 mL of Base (0.5 M KOH)
[16:40] Stepping pH = 3.66
[16:55] Stirrer speed set to 0
[17:05] Datapoint id 9 collected
[17:05] Charge balance equation is out by -8.3%
[17:05] Stirrer speed set to 50
[17:10] pH 3.67 -> 3.87
[17:10] Using charge balance adjust
[17:10] Dispensed 0.000682 mL of Base (0.5 M KOH)
[17:30] Stirrer speed set to 0
[17:41] Datapoint id 10 collected

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[17:41] Charge balance equation is out by 15.6%
[17:41] Stirrer speed set to 50
[17:46] pH 3.91 -> 4.11
[17:46] Using cautious pH adjust
[17:46] Dispensed 0.000353 mL of Base (0.5 M KOH)
[17:51] Stepping pH = 4.02
[17:51] Dispensed 0.000235 mL of Base (0.5 M KOH)
[17:56] Stepping pH = 4.10
[17:56] Dispensed 0.000047 mL of Base (0.5 M KOH)
[18:01] Stepping pH = 4.11
[18:16] Stirrer speed set to 0
[18:26] Datapoint id 11 collected
[18:26] Charge balance equation is out by 11.4%
[18:26] Stirrer speed set to 50
[18:31] pH 4.10 -> 4.30
[18:31] Using charge balance adjust
[18:32] Dispensed 0.000800 mL of Base (0.5 M KOH)
[18:52] Stirrer speed set to 0
[19:02] Datapoint id 12 collected
[19:02] Charge balance equation is out by 29.2%
[19:02] Stirrer speed set to 50
[19:07] pH 4.36 -> 4.56
[19:07] Using cautious pH adjust
[19:07] Dispensed 0.000447 mL of Base (0.5 M KOH)
[19:12] Stepping pH = 4.48
[19:12] Dispensed 0.000259 mL of Base (0.5 M KOH)
[19:17] Stepping pH = 4.55
[19:17] Dispensed 0.000047 mL of Base (0.5 M KOH)
[19:22] Stepping pH = 4.55
[19:22] Dispensed 0.000259 mL of Base (0.5 M KOH)
[19:28] Stepping pH = 4.62
[19:43] Stirrer speed set to 0
[19:54] Datapoint id 13 collected
[19:54] Charge balance equation is out by -12.3%
[19:54] Stirrer speed set to 50
[19:59] pH 4.61 -> 4.81
[19:59] Using charge balance adjust
[19:59] Dispensed 0.000917 mL of Base (0.5 M KOH)
[20:20] Stirrer speed set to 0
[20:35] Datapoint id 14 collected
[20:35] Charge balance equation is out by -8.1%
[20:35] Stirrer speed set to 50
[20:40] pH 4.81 -> 5.01
[20:40] Using charge balance adjust
[20:40] Dispensed 0.000847 mL of Base (0.5 M KOH)
[21:00] Stirrer speed set to 0
[21:13] Datapoint id 15 collected
[21:13] Charge balance equation is out by -18.0%
[21:13] Stirrer speed set to 50
[21:18] pH 5.00 -> 5.20
[21:18] Using cautious pH adjust
[21:18] Dispensed 0.000353 mL of Base (0.5 M KOH)
[21:23] Stepping pH = 5.07
[21:23] Dispensed 0.000376 mL of Base (0.5 M KOH)
[21:28] Stepping pH = 5.17
[21:28] Dispensed 0.000071 mL of Base (0.5 M KOH)
[21:33] Stepping pH = 5.14
[21:33] Dispensed 0.000870 mL of Base (0.5 M KOH)
[21:39] Stepping pH = 5.45

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[21:54] Stirrer speed set to 0
[22:09] Datapoint id 16 collected
[22:09] Charge balance equation is out by -134.1%
[22:09] Stirrer speed set to 50
[22:14] pH 5.41 -> 5.61
[22:14] Using cautious pH adjust
[22:14] Dispensed 0.000212 mL of Base (0.5 M KOH)
[22:19] Stepping pH = 5.41
[22:19] Dispensed 0.001035 mL of Base (0.5 M KOH)
[22:24] Stepping pH = 6.09
[22:39] Stirrer speed set to 0
[23:05] Datapoint id 17 collected
[23:05] Charge balance equation is out by -201.4%
[23:05] Stirrer speed set to 50
[23:10] pH 5.99 -> 6.19
[23:10] Using cautious pH adjust
[23:10] Dispensed 0.000071 mL of Base (0.5 M KOH)
[23:15] Stepping pH = 5.99
[23:15] Dispensed 0.000235 mL of Base (0.5 M KOH)
[23:20] Stepping pH = 6.23
[23:35] Stirrer speed set to 0
[24:01] Datapoint id 18 collected
[24:01] Charge balance equation is out by -98.3%
[24:01] Stirrer speed set to 50
[24:06] pH 6.26 -> 6.46
[24:06] Using cautious pH adjust
[24:06] Dispensed 0.000047 mL of Base (0.5 M KOH)
[24:11] Stepping pH = 6.26
[24:11] Dispensed 0.000165 mL of Base (0.5 M KOH)
[24:16] Stepping pH = 6.37
[24:16] Dispensed 0.000094 mL of Base (0.5 M KOH)
[24:21] Stepping pH = 6.59
[24:37] Stirrer speed set to 0
[25:17] Datapoint id 19 collected
[25:17] Charge balance equation is out by -178.7%
[25:17] Stirrer speed set to 50
[25:22] pH 6.71 -> 6.91
[25:22] Using cautious pH adjust
[25:22] Dispensed 0.000024 mL of Base (0.5 M KOH)
[25:27] Stepping pH = 6.72
[25:27] Dispensed 0.000071 mL of Base (0.5 M KOH)
[25:32] Stepping pH = 6.75
[25:32] Dispensed 0.000165 mL of Base (0.5 M KOH)
[25:37] Stepping pH = 8.75
[25:52] Stirrer speed set to 0
[26:52] Datapoint id 20 collected
[26:52] Charge balance equation is out by -408.8%
[26:52] Stirrer speed set to 50
[26:57] pH 8.97 -> 9.17
[26:57] Using cautious pH adjust
[26:57] Dispensed 0.000024 mL of Base (0.5 M KOH)
[27:03] Stepping pH = 8.97
[27:03] Dispensed 0.000094 mL of Base (0.5 M KOH)
[27:08] Stepping pH = 8.98
[27:08] Dispensed 0.000282 mL of Base (0.5 M KOH)
[27:13] Stepping pH = 9.83
[27:28] Stirrer speed set to 0
[27:45] Datapoint id 21 collected
[27:45] Charge balance equation is out by -942.4%

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[27:45] Stirrer speed set to 50
[27:50] pH 9.85 -> 10.05
[27:50] Using cautious pH adjust
[27:50] Dispensed 0.000118 mL of Base (0.5 M KOH)
[27:55] Stepping pH = 9.87
[27:55] Dispensed 0.000259 mL of Base (0.5 M KOH)
[28:00] Stepping pH = 10.13
[28:15] Stirrer speed set to 0
[28:34] Datapoint id 22 collected
[28:34] Charge balance equation is out by -73.7%
[28:34] Titration 2 of 3
[28:34] Adding initial titrants
[28:34] Automatically add 0.05000 mL of Octanol
[28:35] Dispensed 0.050000 mL of Octanol
[28:35] Stirrer speed set to 10
[28:36] Stirrer speed set to 55
[28:36] Iterative adjust 10.14 -> 2.00
[28:36] pH 10.14 -> 2.00
[28:37] Dispensed 0.052658 mL of Acid (0.5 M HCl)
[28:42] pH 2.02 -> 2.00
[28:43] Dispensed 0.001976 mL of Acid (0.5 M HCl)
[29:33] Stirrer speed set to 0
[29:43] Datapoint id 23 collected
[29:43] Stirrer speed set to 55
[29:48] pH 1.97 -> 2.17
[29:48] Using cautious pH adjust
[29:49] Dispensed 0.009196 mL of Base (0.5 M KOH)
[29:54] Stepping pH = 2.06
[29:54] Dispensed 0.006515 mL of Base (0.5 M KOH)
[29:59] Stepping pH = 2.14
[29:59] Dispensed 0.001505 mL of Base (0.5 M KOH)
[30:04] Stepping pH = 2.16
[30:20] Stirrer speed set to 0
[30:30] Datapoint id 24 collected
[30:30] Charge balance equation is out by 6.5%
[30:30] Stirrer speed set to 55
[30:35] pH 2.16 -> 2.36
[30:35] Using charge balance adjust
[30:36] Dispensed 0.011618 mL of Base (0.5 M KOH)
[30:56] Stirrer speed set to 0
[31:06] Datapoint id 25 collected
[31:06] Charge balance equation is out by 20.5%
[31:06] Stirrer speed set to 55
[31:11] pH 2.41 -> 2.61
[31:11] Using cautious pH adjust
[31:11] Dispensed 0.003293 mL of Base (0.5 M KOH)
[31:16] Stepping pH = 2.51
[31:16] Dispensed 0.002023 mL of Base (0.5 M KOH)
[31:21] Stepping pH = 2.58
[31:21] Dispensed 0.000823 mL of Base (0.5 M KOH)
[31:27] Stepping pH = 2.60
[31:42] Stirrer speed set to 0
[31:52] Datapoint id 26 collected
[31:52] Charge balance equation is out by 6.8%
[31:52] Stirrer speed set to 55
[31:57] pH 2.61 -> 2.81
[31:57] Using charge balance adjust
[31:57] Dispensed 0.004257 mL of Base (0.5 M KOH)
[32:17] Stirrer speed set to 0

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[32:27] Datapoint id 27 collected
[32:27] Charge balance equation is out by 11.6%
[32:27] Stirrer speed set to 55
[32:32] pH 2.83 -> 3.03
[32:32] Using charge balance adjust
[32:32] Dispensed 0.002634 mL of Base (0.5 M KOH)
[32:53] Stirrer speed set to 0
[33:03] Datapoint id 28 collected
[33:03] Charge balance equation is out by 26.9%
[33:03] Stirrer speed set to 55
[33:08] pH 3.09 -> 3.29
[33:08] Using cautious pH adjust
[33:08] Dispensed 0.000823 mL of Base (0.5 M KOH)
[33:13] Stepping pH = 3.19
[33:13] Dispensed 0.000588 mL of Base (0.5 M KOH)
[33:18] Stepping pH = 3.27
[33:18] Dispensed 0.000118 mL of Base (0.5 M KOH)
[33:23] Stepping pH = 3.28
[33:23] Dispensed 0.000094 mL of Base (0.5 M KOH)
[33:28] Stepping pH = 3.30
[33:44] Stirrer speed set to 0
[33:54] Datapoint id 29 collected
[33:54] Charge balance equation is out by 1.7%
[33:54] Stirrer speed set to 55
[33:59] pH 3.30 -> 3.50
[33:59] Using charge balance adjust
[33:59] Dispensed 0.001246 mL of Base (0.5 M KOH)
[34:19] Stirrer speed set to 0
[34:29] Datapoint id 30 collected
[34:29] Charge balance equation is out by -0.4%
[34:29] Stirrer speed set to 55
[34:34] pH 3.51 -> 3.71
[34:34] Using charge balance adjust
[34:34] Dispensed 0.001105 mL of Base (0.5 M KOH)
[34:54] Stirrer speed set to 0
[35:05] Datapoint id 31 collected
[35:05] Charge balance equation is out by 1.1%
[35:05] Stirrer speed set to 55
[35:10] pH 3.71 -> 3.91
[35:10] Using charge balance adjust
[35:10] Dispensed 0.001058 mL of Base (0.5 M KOH)
[35:30] Stirrer speed set to 0
[35:40] Datapoint id 32 collected
[35:40] Charge balance equation is out by 2.5%
[35:40] Stirrer speed set to 55
[35:45] pH 3.92 -> 4.12
[35:45] Using charge balance adjust
[35:46] Dispensed 0.001058 mL of Base (0.5 M KOH)
[36:06] Stirrer speed set to 0
[36:16] Datapoint id 33 collected
[36:16] Charge balance equation is out by 3.6%
[36:16] Stirrer speed set to 55
[36:21] pH 4.13 -> 4.33
[36:21] Using charge balance adjust
[36:21] Dispensed 0.001011 mL of Base (0.5 M KOH)
[36:41] Stirrer speed set to 0
[36:51] Datapoint id 34 collected
[36:51] Charge balance equation is out by -3.3%
[36:51] Stirrer speed set to 55

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[36:56] pH 4.34 -> 4.54
[36:56] Using charge balance adjust
[36:56] Dispensed 0.000894 mL of Base (0.5 M KOH)
[37:17] Stirrer speed set to 0
[37:27] Datapoint id 35 collected
[37:27] Charge balance equation is out by -9.8%
[37:27] Stirrer speed set to 55
[37:32] pH 4.53 -> 4.73
[37:32] Using charge balance adjust
[37:32] Dispensed 0.000753 mL of Base (0.5 M KOH)
[37:53] Stirrer speed set to 0
[38:03] Datapoint id 36 collected
[38:03] Charge balance equation is out by -11.7%
[38:03] Stirrer speed set to 55
[38:08] pH 4.72 -> 4.92
[38:08] Using charge balance adjust
[38:08] Dispensed 0.000588 mL of Base (0.5 M KOH)
[38:29] Stirrer speed set to 0
[38:39] Datapoint id 37 collected
[38:39] Charge balance equation is out by -30.8%
[38:39] Stirrer speed set to 55
[38:44] pH 4.87 -> 5.07
[38:44] Using cautious pH adjust
[38:44] Dispensed 0.000235 mL of Base (0.5 M KOH)
[38:49] Stepping pH = 4.93
[38:49] Dispensed 0.000282 mL of Base (0.5 M KOH)
[38:54] Stepping pH = 5.01
[38:55] Dispensed 0.000141 mL of Base (0.5 M KOH)
[39:00] Stepping pH = 5.05
[39:00] Dispensed 0.000071 mL of Base (0.5 M KOH)
[39:05] Stepping pH = 5.07
[39:20] Stirrer speed set to 0
[39:30] Datapoint id 38 collected
[39:30] Charge balance equation is out by -55.1%
[39:30] Stirrer speed set to 55
[39:36] pH 5.09 -> 5.29
[39:36] Using cautious pH adjust
[39:36] Dispensed 0.000165 mL of Base (0.5 M KOH)
[39:41] Stepping pH = 5.13
[39:41] Dispensed 0.000282 mL of Base (0.5 M KOH)
[39:46] Stepping pH = 5.28
[39:46] Dispensed 0.000024 mL of Base (0.5 M KOH)
[39:51] Stepping pH = 5.29
[40:06] Stirrer speed set to 0
[40:18] Datapoint id 39 collected
[40:18] Charge balance equation is out by -46.4%
[40:18] Stirrer speed set to 55
[40:23] pH 5.30 -> 5.50
[40:23] Using cautious pH adjust
[40:23] Dispensed 0.000118 mL of Base (0.5 M KOH)
[40:28] Stepping pH = 5.32
[40:28] Dispensed 0.000282 mL of Base (0.5 M KOH)
[40:33] Stepping pH = 5.58
[40:48] Stirrer speed set to 0
[41:00] Datapoint id 40 collected
[41:00] Charge balance equation is out by -83.4%
[41:00] Stirrer speed set to 55
[41:05] pH 5.62 -> 5.82
[41:05] Using cautious pH adjust

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[41:05] Dispensed 0.000071 mL of Base (0.5 M KOH)
[41:11] Stepping pH = 5.63
[41:11] Dispensed 0.000188 mL of Base (0.5 M KOH)
[41:16] Stepping pH = 5.66
[41:16] Dispensed 0.000376 mL of Base (0.5 M KOH)
[41:21] Stepping pH = 6.69
[41:36] Stirrer speed set to 0
[42:36] Datapoint id 41 collected
[42:36] Charge balance equation is out by -392.1%
[42:36] Stirrer speed set to 55
[42:41] pH 6.97 -> 7.17
[42:41] Using cautious pH adjust
[42:41] Dispensed 0.000024 mL of Base (0.5 M KOH)
[42:46] Stepping pH = 7.02
[42:46] Dispensed 0.000024 mL of Base (0.5 M KOH)
[42:51] Stepping pH = 7.05
[42:51] Dispensed 0.000024 mL of Base (0.5 M KOH)
[42:56] Stepping pH = 7.08
[42:56] Dispensed 0.000047 mL of Base (0.5 M KOH)
[43:02] Stepping pH = 7.10
[43:02] Dispensed 0.000047 mL of Base (0.5 M KOH)
[43:07] Stepping pH = 7.10
[43:07] Dispensed 0.000282 mL of Base (0.5 M KOH)
[43:12] Stepping pH = 9.27
[43:27] Stirrer speed set to 0
[43:45] Datapoint id 42 collected
[43:45] Charge balance equation is out by -1,782.6%
[43:45] Stirrer speed set to 55
[43:50] pH 9.30 -> 9.50
[43:50] Using cautious pH adjust
[43:50] Dispensed 0.000047 mL of Base (0.5 M KOH)
[43:56] Stepping pH = 9.30
[43:56] Dispensed 0.000212 mL of Base (0.5 M KOH)
[44:01] Stepping pH = 9.60
[44:16] Stirrer speed set to 0
[44:37] Datapoint id 43 collected
[44:37] Charge balance equation is out by -200.1%
[44:37] Stirrer speed set to 55
[44:42] pH 9.58 -> 9.78
[44:42] Using cautious pH adjust
[44:42] Dispensed 0.000071 mL of Base (0.5 M KOH)
[44:47] Stepping pH = 9.58
[44:47] Dispensed 0.000353 mL of Base (0.5 M KOH)
[44:52] Stepping pH = 9.97
[45:07] Stirrer speed set to 0
[45:21] Datapoint id 44 collected
[45:21] Charge balance equation is out by -201.1%
[45:21] Stirrer speed set to 55
[45:26] pH 9.95 -> 10.05
[45:26] Using cautious pH adjust
[45:26] Dispensed 0.000071 mL of Base (0.5 M KOH)
[45:31] Stepping pH = 9.94
[45:31] Dispensed 0.000329 mL of Base (0.5 M KOH)
[45:36] Stepping pH = 10.17
[45:51] Stirrer speed set to 0
[46:01] Datapoint id 45 collected
[46:01] Charge balance equation is out by -210.8%
[46:01] Titration 3 of 3
[46:01] Adding initial titrants

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[46:01] Automatically add 0.25000 mL of Octanol
[46:07] Dispensed 0.250000 mL of Octanol
[46:07] Stirrer speed set to 10
[46:08] Stirrer speed set to 60
[46:08] Iterative adjust 10.17 -> 2.00
[46:08] pH 10.17 -> 2.00
[46:10] Dispensed 0.055715 mL of Acid (0.5 M HCl)
[46:15] pH 2.03 -> 2.00
[46:15] Dispensed 0.003457 mL of Acid (0.5 M HCl)
[47:05] Stirrer speed set to 0
[47:15] Datapoint id 46 collected
[47:15] Stirrer speed set to 60
[47:20] pH 1.96 -> 2.16
[47:20] Using cautious pH adjust
[47:21] Dispensed 0.010113 mL of Base (0.5 M KOH)
[47:26] Stepping pH = 2.02
[47:26] Dispensed 0.010865 mL of Base (0.5 M KOH)
[47:31] Stepping pH = 2.09
[47:31] Dispensed 0.006515 mL of Base (0.5 M KOH)
[47:36] Stepping pH = 2.18
[47:51] Stirrer speed set to 0
[48:01] Datapoint id 47 collected
[48:01] Charge balance equation is out by -35.9%
[48:01] Stirrer speed set to 60
[48:06] pH 2.19 -> 2.39
[48:06] Using cautious pH adjust
[48:07] Dispensed 0.005903 mL of Base (0.5 M KOH)
[48:12] Stepping pH = 2.29
[48:12] Dispensed 0.003481 mL of Base (0.5 M KOH)
[48:17] Stepping pH = 2.36
[48:17] Dispensed 0.001435 mL of Base (0.5 M KOH)
[48:22] Stepping pH = 2.39
[48:37] Stirrer speed set to 0
[48:47] Datapoint id 48 collected
[48:47] Charge balance equation is out by 8.3%
[48:47] Stirrer speed set to 60
[48:52] pH 2.39 -> 2.59
[48:52] Using charge balance adjust
[48:53] Dispensed 0.007502 mL of Base (0.5 M KOH)
[49:13] Stirrer speed set to 0
[49:23] Datapoint id 49 collected
[49:23] Charge balance equation is out by 9.3%
[49:23] Stirrer speed set to 60
[49:28] pH 2.62 -> 2.82
[49:28] Using charge balance adjust
[49:28] Dispensed 0.004657 mL of Base (0.5 M KOH)
[49:48] Stirrer speed set to 0
[49:59] Datapoint id 50 collected
[49:59] Charge balance equation is out by 13.0%
[49:59] Stirrer speed set to 60
[50:04] pH 2.85 -> 3.05
[50:04] Using charge balance adjust
[50:04] Dispensed 0.002987 mL of Base (0.5 M KOH)
[50:24] Stirrer speed set to 0
[50:34] Datapoint id 51 collected
[50:34] Charge balance equation is out by 15.0%
[50:34] Stirrer speed set to 60
[50:39] pH 3.08 -> 3.28
[50:39] Using cautious pH adjust

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[50:39] Dispensed 0.001058 mL of Base (0.5 M KOH)
[50:44] Stepping pH = 3.17
[50:44] Dispensed 0.000823 mL of Base (0.5 M KOH)
[50:50] Stepping pH = 3.24
[50:50] Dispensed 0.000329 mL of Base (0.5 M KOH)
[50:55] Stepping pH = 3.27
[51:10] Stirrer speed set to 0
[51:20] Datapoint id 52 collected
[51:20] Charge balance equation is out by -4.5%
[51:20] Stirrer speed set to 60
[51:25] pH 3.28 -> 3.48
[51:25] Using charge balance adjust
[51:25] Dispensed 0.001717 mL of Base (0.5 M KOH)
[51:45] Stirrer speed set to 0
[51:55] Datapoint id 53 collected
[51:55] Charge balance equation is out by -5.2%
[51:55] Stirrer speed set to 60
[52:00] pH 3.47 -> 3.67
[52:00] Using charge balance adjust
[52:00] Dispensed 0.001458 mL of Base (0.5 M KOH)
[52:21] Stirrer speed set to 0
[52:31] Datapoint id 54 collected
[52:31] Charge balance equation is out by -0.7%
[52:31] Stirrer speed set to 60
[52:36] pH 3.68 -> 3.88
[52:36] Using charge balance adjust
[52:36] Dispensed 0.001246 mL of Base (0.5 M KOH)
[52:56] Stirrer speed set to 0
[53:06] Datapoint id 55 collected
[53:06] Charge balance equation is out by 3.3%
[53:06] Stirrer speed set to 60
[53:11] pH 3.89 -> 4.09
[53:11] Using charge balance adjust
[53:11] Dispensed 0.001011 mL of Base (0.5 M KOH)
[53:31] Stirrer speed set to 0
[53:41] Datapoint id 56 collected
[53:41] Charge balance equation is out by -1.8%
[53:41] Stirrer speed set to 60
[53:47] pH 4.10 -> 4.30
[53:47] Using charge balance adjust
[53:47] Dispensed 0.000800 mL of Base (0.5 M KOH)
[54:07] Stirrer speed set to 0
[54:17] Datapoint id 57 collected
[54:17] Charge balance equation is out by -9.4%
[54:17] Stirrer speed set to 60
[54:22] pH 4.29 -> 4.49
[54:22] Using charge balance adjust
[54:22] Dispensed 0.000588 mL of Base (0.5 M KOH)
[54:42] Stirrer speed set to 0
[54:52] Datapoint id 58 collected
[54:52] Charge balance equation is out by -20.0%
[54:52] Stirrer speed set to 60
[54:57] pH 4.45 -> 4.65
[54:57] Using cautious pH adjust
[54:57] Dispensed 0.000235 mL of Base (0.5 M KOH)
[55:02] Stepping pH = 4.52
[55:02] Dispensed 0.000235 mL of Base (0.5 M KOH)
[55:08] Stepping pH = 4.61
[55:08] Dispensed 0.000094 mL of Base (0.5 M KOH)

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[55:13] Stepping pH = 4.62
[55:13] Dispensed 0.000118 mL of Base (0.5 M KOH)
[55:18] Stepping pH = 4.67
[55:33] Stirrer speed set to 0
[55:43] Datapoint id 59 collected
[55:43] Charge balance equation is out by -49.9%
[55:43] Stirrer speed set to 60
[55:49] pH 4.68 -> 4.88
[55:49] Using cautious pH adjust
[55:49] Dispensed 0.000141 mL of Base (0.5 M KOH)
[55:54] Stepping pH = 4.75
[55:54] Dispensed 0.000165 mL of Base (0.5 M KOH)
[55:59] Stepping pH = 4.86
[55:59] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:04] Stepping pH = 4.86
[56:04] Dispensed 0.000094 mL of Base (0.5 M KOH)
[56:09] Stepping pH = 4.92
[56:24] Stirrer speed set to 0
[56:35] Datapoint id 60 collected
[56:35] Charge balance equation is out by -46.6%
[56:35] Stirrer speed set to 60
[56:40] pH 4.93 -> 5.13
[56:40] Using cautious pH adjust
[56:40] Dispensed 0.000094 mL of Base (0.5 M KOH)
[56:45] Stepping pH = 4.97
[56:45] Dispensed 0.000165 mL of Base (0.5 M KOH)
[56:50] Stepping pH = 5.15
[57:05] Stirrer speed set to 0
[57:16] Datapoint id 61 collected
[57:16] Charge balance equation is out by -38.7%
[57:16] Stirrer speed set to 60
[57:21] pH 5.16 -> 5.36
[57:21] Using cautious pH adjust
[57:21] Dispensed 0.000047 mL of Base (0.5 M KOH)
[57:27] Stepping pH = 5.17
[57:27] Dispensed 0.000165 mL of Base (0.5 M KOH)
[57:32] Stepping pH = 5.35
[57:47] Stirrer speed set to 0
[57:58] Datapoint id 62 collected
[57:58] Charge balance equation is out by -87.8%
[57:58] Stirrer speed set to 60
[58:03] pH 5.38 -> 5.58
[58:03] Using cautious pH adjust
[58:03] Dispensed 0.000047 mL of Base (0.5 M KOH)
[58:09] Stepping pH = 5.41
[58:09] Dispensed 0.000094 mL of Base (0.5 M KOH)
[58:14] Stepping pH = 5.54
[58:14] Dispensed 0.000024 mL of Base (0.5 M KOH)
[58:19] Stepping pH = 5.57
[58:34] Stirrer speed set to 0
[58:47] Datapoint id 63 collected
[58:47] Charge balance equation is out by -84.7%
[58:47] Stirrer speed set to 60
[58:52] pH 5.63 -> 5.83
[58:52] Using cautious pH adjust
[58:52] Dispensed 0.000024 mL of Base (0.5 M KOH)
[58:57] Stepping pH = 5.64
[58:57] Dispensed 0.000094 mL of Base (0.5 M KOH)
[59:02] Stepping pH = 5.74

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[59:02] Dispensed 0.000047 mL of Base (0.5 M KOH)
[59:07] Stepping pH = 5.86
[59:22] Stirrer speed set to 0
[59:58] Datapoint id 64 collected
[59:58] Charge balance equation is out by -167.1%
[59:58] Stirrer speed set to 60
[1:00:03] pH 5.99 -> 6.19
[1:00:03] Using cautious pH adjust
[1:00:03] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:00:08] Stepping pH = 6.02
[1:00:08] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:00:13] Stepping pH = 6.15
[1:00:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:00:18] Stepping pH = 6.30
[1:00:33] Stirrer speed set to 0
[1:01:33] Datapoint id 65 collected
[1:01:33] Charge balance equation is out by -96.8%
[1:01:33] Stirrer speed set to 60
[1:01:38] pH 6.35 -> 6.55
[1:01:38] Using cautious pH adjust
[1:01:38] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:43] Stepping pH = 6.40
[1:01:43] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:01:48] Stepping pH = 6.63
[1:02:04] Stirrer speed set to 0
[1:03:04] Datapoint id 66 collected
[1:03:04] Charge balance equation is out by -27.0%
[1:03:04] Stirrer speed set to 60
[1:03:09] pH 6.73 -> 6.93
[1:03:09] Using cautious pH adjust
[1:03:09] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:03:14] Stepping pH = 6.79
[1:03:14] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:03:19] Stepping pH = 7.01
[1:03:34] Stirrer speed set to 0
[1:04:34] Datapoint id 67 collected
[1:04:34] Charge balance equation is out by -13.9%
[1:04:34] Stirrer speed set to 60
[1:04:39] pH 7.04 -> 7.24
[1:04:39] Using charge balance adjust
[1:04:39] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:04:59] Stirrer speed set to 0
[1:05:59] Datapoint id 68 collected
[1:05:59] Charge balance equation is out by -70.5%
[1:05:59] Stirrer speed set to 60
[1:06:05] pH 7.21 -> 7.41
[1:06:05] Using cautious pH adjust
[1:06:05] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:06:10] Stepping pH = 7.21
[1:06:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:06:15] Stepping pH = 7.44
[1:06:30] Stirrer speed set to 0
[1:07:30] Datapoint id 69 collected
[1:07:30] Charge balance equation is out by -155.1%
[1:07:30] Stirrer speed set to 60
[1:07:35] pH 7.73 -> 7.93
[1:07:35] Using cautious pH adjust
[1:07:35] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:07:40] Stepping pH = 7.83

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:07:40] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:07:45] Stepping pH = 8.04
[1:08:00] Stirrer speed set to 0
[1:09:00] Datapoint id 70 collected
[1:09:00] Charge balance equation is out by -346.1%
[1:09:00] Stirrer speed set to 60
[1:09:06] pH 7.76 -> 7.96
[1:09:06] Using cautious pH adjust
[1:09:06] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:09:11] Stepping pH = 7.79
[1:09:11] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:09:16] Stepping pH = 8.01
[1:09:31] Stirrer speed set to 0
[1:10:31] Datapoint id 71 collected
[1:10:31] Charge balance equation is out by -354.4%
[1:10:31] Stirrer speed set to 60
[1:10:36] pH 8.11 -> 8.31
[1:10:36] Using cautious pH adjust
[1:10:36] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:10:41] Stepping pH = 8.17
[1:10:41] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:10:46] Stepping pH = 8.19
[1:10:46] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:10:51] Stepping pH = 8.17
[1:10:51] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:10:57] Stepping pH = 8.47
[1:11:12] Stirrer speed set to 0
[1:12:12] Datapoint id 72 collected
[1:12:12] Charge balance equation is out by -1,435.6%
[1:12:12] Stirrer speed set to 60
[1:12:17] pH 8.43 -> 8.63
[1:12:17] Using cautious pH adjust
[1:12:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:12:22] Stepping pH = 8.42
[1:12:22] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:12:27] Stepping pH = 8.45
[1:12:27] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:12:32] Stepping pH = 8.81
[1:12:47] Stirrer speed set to 0
[1:13:08] Datapoint id 73 collected
[1:13:08] Charge balance equation is out by -948.3%
[1:13:08] Stirrer speed set to 60
[1:13:13] pH 8.83 -> 9.03
[1:13:13] Using cautious pH adjust
[1:13:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:13:18] Stepping pH = 8.84
[1:13:18] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:13:23] Stepping pH = 8.94
[1:13:23] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:13:28] Stepping pH = 9.00
[1:13:28] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:13:33] Stepping pH = 9.04
[1:13:49] Stirrer speed set to 0
[1:14:02] Datapoint id 74 collected
[1:14:02] Charge balance equation is out by -262.5%
[1:14:02] Stirrer speed set to 60
[1:14:07] pH 9.05 -> 9.25
[1:14:07] Using cautious pH adjust
[1:14:07] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M07_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28011**
Filename: **C:\Sirius_T3\Mehtap\20180228_exp28_logP_T3-2\18B-28011_M07_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 4:26:20 PM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:14:13] Stepping pH = 9.04
[1:14:13] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:14:18] Stepping pH = 9.33
[1:14:33] Stirrer speed set to 0
[1:14:50] Datapoint id 75 collected
[1:14:50] Charge balance equation is out by -206.3%
[1:14:50] Stirrer speed set to 60
[1:14:55] pH 9.34 -> 9.54
[1:14:55] Using cautious pH adjust
[1:14:56] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:15:01] Stepping pH = 9.37
[1:15:01] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:15:06] Stepping pH = 9.53
[1:15:21] Stirrer speed set to 0
[1:15:31] Datapoint id 76 collected
[1:15:31] Charge balance equation is out by -78.6%
[1:15:31] Stirrer speed set to 60
[1:15:37] pH 9.54 -> 9.74
[1:15:37] Using cautious pH adjust
[1:15:37] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:15:42] Stepping pH = 9.57
[1:15:42] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:15:47] Stepping pH = 9.72
[1:15:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:15:52] Stepping pH = 9.73
[1:16:07] Stirrer speed set to 0
[1:16:18] Datapoint id 77 collected
[1:16:18] Charge balance equation is out by -62.5%
[1:16:18] Stirrer speed set to 60
[1:16:23] pH 9.73 -> 9.93
[1:16:23] Using cautious pH adjust
[1:16:23] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:16:28] Stepping pH = 9.78
[1:16:28] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:16:33] Stepping pH = 9.93
[1:16:48] Stirrer speed set to 0
[1:16:59] Datapoint id 78 collected
[1:16:59] Charge balance equation is out by -29.9%
[1:16:59] Stirrer speed set to 60
[1:17:04] pH 9.92 -> 10.05
[1:17:04] Using cautious pH adjust
[1:17:04] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:17:09] Stepping pH = 9.95
[1:17:09] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:17:14] Stepping pH = 10.04
[1:17:29] Stirrer speed set to 0
[1:17:42] Datapoint id 79 collected
[1:17:42] Charge balance equation is out by -36.7%
[1:17:42] Argon flow rate set to 0
[1:17:46] Titrator arm moved over Titration position